Lanczos tridiagonalization, Golub-Kahan bidiagonalization and core problem

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1 Introduction

Consider an orthogonally invariant linear approximation problem \( Ax \approx b \). In [8] it is proved that the partial upper bidiagonalization of the extended matrix \([b, A]\) determines a core approximation problem \( A_{11} x_1 \approx b_1 \), with all necessary and sufficient information for solving the original problem given by \( b_1 \) and \( A_{11} \). It is shown how the core problem can be used in a simple and efficient way for solving different formulations of the original approximation problems. In [3] the core problem formulation is derived from the relationship between the Golub-Kahan bidiagonalization [2] and the Lanczos tridiagonalization [5], and from the known properties of Jacobi matrices. Here we briefly recall the approach from [3], and outline a possible direction for further research.

2 Core problem

Consider estimating \( x \) from the real linear approximation problem

\[
Ax \approx b, \quad A \text{ a nonzero } n \text{ by } m \text{ matrix, } \quad b \text{ a nonzero } n \text{-vector},
\]

where the uninteresting case is excluded by the assumption \( A^T b \neq 0 \). In the paper [8] it was proposed to transform the original data \([b, A]\) into the form

\[
P^T \left[ \begin{array}{ccc} b_1 & \ldots & 0 \\ 0 & \ldots & A_{22} \end{array} \right], \quad \text{where } \quad P^{-1} = P^T, \quad Q^{-1} = Q^T,
\]

(2)

where \( b_1 = \beta_1 e_1 \) and \( A_{11} \) is a lower bidiagonal matrix with nonzero bidiagonal elements. The matrix \( A_{11} \) is either square, when \( (1) \) is compatible, or rectangular, when \( (1) \) is incompatible. The original problem is in this way decomposed into the approximation problems \( A_{11} x_1 \approx b_1 \) and \( A_{22} x_2 \approx 0 \). It is suggested to solve the first problem, set \( x_2 \equiv 0 \) and substitute \( x \equiv Q^T[A_x^T, 0]^T \) for the solution of \( (1) \). The transformation described above has the following remarkable properties, see [3, Theorem 1.1], with the proof given in [8, Theorem 2.2, 3.2, 3.3].

**Theorem 2.1** Let \( A \) be a nonzero \( n \) by \( m \) real matrix and \( b \) a nonzero real \( n \)-vector, \( A^T b \neq 0 \). Then there exists a decomposition (2), where \( b_1 = \beta_1 e_1 \) and \( A_{11} \) is a lower bidiagonal matrix with nonzero bidiagonal elements. Moreover:

1. The matrix \( A_{11} \) has full column rank and its singular values are simple.
2. The matrix \( A_{11} \) has minimal dimensions over all orthogonal transformations giving the block structure (2).
3. All components of \( b_1 = \beta_1 e_1 \) in the left singular vector subspaces of \( A_{11} \) are nonzero.

The proof of Theorem 2.1 in [8] is based on the singular value decomposition of the matrix \( A \). In [3] the relationship between the Golub-Kahan bidiagonalization and the Lanczos tridiagonalization is used for constructing the proof.

3 Lanczos tridiagonalization and core problem properties

Consider the partial lower Golub-Kahan bidiagonalization of \([b, A]\) in the following form. Given the initial vectors \( v_0 \equiv 0, u_1 \equiv b/\beta_1 \), where \( \beta_1 \equiv ||b|| \neq 0 \) and \( ||.|| \) represents the standard Euclidean norm, the algorithm computes for \( i = 1, 2, \ldots \)

\[
\beta_i v_i = A^T u_i - \beta_i v_{i-1}, \quad ||v_i|| = 1, \quad \beta_{i+1} u_{i+1} = A v_i - \alpha_i u_i, \quad ||u_{i+1}|| = 1
\]

(3)

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until $\alpha_i = 0$ or $\beta_{k+1} = 0$, or until $i = \min\{n, m\}$. Denote $U_k \equiv (u_1, \ldots, u_k)$, $V_k \equiv (v_1, \ldots, v_k)$ the matrices with orthonormal columns, $L_k$ the square lower bidiagonal matrix with the main diagonal $(\alpha_1, \ldots, \alpha_k)$ and the subdiagonal $(\beta_2, \ldots, \beta_k)$ and $L_{k+1} \equiv (L_k^T, \beta_{k+1} e_k)^T$. In the rest of this contribution we consider (1) incompatible; the compatible case is simpler and can be treated analogously, see [3]. Then (3) must stop with some $\alpha_{p+1} = 0$ or $p = m$ giving

$$A^T U_p = V_p L_p^T, \quad AV_p = U_{p+1} L_{p+1}.$$  

Consequently, $U_{p+1}^T [b, AV_p] = [\beta_1 e_1, L_{p+1}^T] \equiv [b_1 | A_{11}]$ and $A_{11} x_1 \equiv L_{p+1} x_1 \approx \beta_1 e_1 \equiv b_1$ is the incompatible core problem. The matrices $U_{p+1}$ and $V_p$ represent the first $(p+1)$ and $p$ columns of the matrices $P$ and $Q$, respectively.

Given a real symmetric matrix $B$ and a starting vector $w_1$, $\|w_1\| = 1$, the Lanczos tridiagonalization algorithm can be written in the matrix form

$$B W_k = W_k T_k + \delta_{k+1} w_{k+1} e_k^T, \quad W_k^T w_{k+1} = 0,$$  

where $W_k e_1 = w_1$, $W_k$ has orthonormal columns and $T_k$ is a symmetric tridiagonal matrix with positive subdiagonal elements, a Jacobi matrix. Defining $B \equiv A^T A$, $w_1 \equiv v_1 = A^T b/\|A^T b\|$, it can be shown (see, e.g., [1]) that the Lanczos tridiagonalization (4) produces the matrices $W_k \equiv V_k$, $T_k \equiv L_{k+1}^2 L_{k+1}$ and $\delta_{k+1} \equiv \alpha_{k+1} \beta_{k+1}$. Thus, the matrix $L_{p+1}$ can be linked to the Jacobi matrix

$$T_p \equiv L_{p+1}^2 L_{p+1} = \begin{pmatrix} \alpha_1^2 + \beta_2^2 & \alpha_2 \beta_2 \\ \alpha_2 \beta_2 & \alpha_2^2 + \beta_3^2 \\ \vdots & \ddots \\ \alpha_p \beta_p & \alpha_p^2 + \beta_{p+1}^2 \end{pmatrix} ; \quad L_{p+1} = \begin{pmatrix} \alpha_1 \\ \beta_2 \\ \vdots \\ \beta_p \\ \alpha_{p+1} \end{pmatrix}.$$  

This fact is used in [3], together with the properties of Jacobi matrices (see, e.g., [9]), for proving Theorem 2.1.

The presented relationship may be found useful in applications of the core problem formulation. In large ill-posed problems the outer Golub-Kahan bidiagonalization can be combined with an inner regularization applied to the problem $L_{k+p} y \approx \beta_k e_1$. Here stopping criteria are typically based on estimation of the L-curve, the discrepancy principle or generalized cross validation (see, e.g., [6], [7]). From the core problem point of view one should ask whether and when the matrix $L_{k+p}$ for $k < p$ (possibly $k < p$) can be considered a sufficiently good approximation to the core matrix $L_{p+1}$. When $p \ll m$, one must ask how to numerically indicate the separation of the core problem, since in finite precision computation $\alpha_{p+1}$ will hardly be identically zero. Similarly, one can ask when the tridiagonal matrix $T_k$, $k < p$, sufficiently approximates the matrix $T_p$ discussed above. It might be useful to study in this context perturbation theory of Jacobi matrices, in particular the specific perturbations when the off-diagonal element $\delta_{k+1} = \alpha_{k+1} \beta_{k+1}$ is replaced by zero, see [4].

We believe that the presented relationships, together with known results on Jacobi matrices, can be used in further investigation of effective stopping criteria in regularization methods.

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