BAND GENERALIZATION OF THE GOLUB–KAHAN BIDIAGONALIZATION, GENERALIZED JACOBI MATRICES, AND THE CORE PROBLEM[*]

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Abstract. The concept of the core problem in total least squares (TLS) problems was introduced in [C. C. Paige and Z. Strakoš, *SIAM J. Matrix Anal. Appl.*, 27, 2006, pp. 861–875]. It is based on orthogonal transformations such that the resulting problem decomposes into two independent parts, with one of the parts having trivial (zero) right-hand side and maximal dimensions, and the other part with nonzero right-hand side having minimal dimensions. Extension of this concept to the multiple right-hand sides case $AX \approx B$ in [I. Hnětynková, M. Plešinger, and Z. Strakoš, *SIAM J. Matrix Anal. Appl.*, 34, 2013, pp. 917–931], which is highly nontrivial, is based on application of the singular value decomposition. In this paper we prove that the band generalization of the Golub–Kahan bidiagonalization proposed in this context by Å. Björck also yields the core problem. We introduce generalized Jacobi matrices and investigate their properties. They prove useful in further analysis of the core problem concept. This paper assumes exact arithmetic.

Key words. total least squares problem, multiple right-hand sides, core problem, Golub–Kahan bidiagonalization, generalized Jacobi matrices.

AMS subject classifications. 15A06, 15A18, 15A21, 15A24, 65F20, 65F25.

1. Introduction.

This paper further elaborates on extending the core problem concept to total least squares problems with multiple right-hand sides; see [13]. We will use the same notations as in [13] and very briefly recall some basic facts. Consider a linear approximation problem

$$AX \approx B, \qquad \text{or, equivalently,} \qquad [B|A] \begin{bmatrix} -I_d \\ X \end{bmatrix} \approx 0, \tag{1.1}$$

where $A \in \mathbb{R}^{m\times n}$, $X \in \mathbb{R}^{n\times d}$, $B \in \mathbb{R}^{m\times d}$, and $A^T B \neq 0$, without any further assumption on the positive integers m, n, d. The matrices A, B, $[B|A]$, and X are called the *system matrix*, the *right-hand side (or the observation) matrix*, the *extended (or data) matrix*, and the *matrix of unknowns*, respectively. We will focus on incompatible problems, i.e., $\mathcal{R}(B) \not\subset \mathcal{R}(A)$, although, the compatible case is not strictly excluded. Consider the orthogonal transformations

$$\widehat{A}\widehat{X} \equiv (P^T A Q)(Q^T X R) \approx (P^T B R) \equiv \widehat{B}, \tag{1.2}$$

where $P^{-1} = P^T$, $Q^{-1} = Q^T$, $R^{-1} = R^T$; or, equivalently,

$$[\widehat{B}|\widehat{A}] \begin{bmatrix} -I_d \\ \widehat{X} \end{bmatrix} \equiv \left(P^T [B|A] \begin{bmatrix} R & 0 \\ 0 & Q \end{bmatrix} \right) \left(\begin{bmatrix} R^T & 0 \\ 0 & Q^T \end{bmatrix} \begin{bmatrix} -I_d \\ X \end{bmatrix} R \right) \approx 0. \tag{1.3}$$

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We call problems (1.1) and (1.2)–(1.3) *orthogonally invariant* and require that X solves (1.1) if and only if $\widehat{X} = Q^T X R$ solves (1.2)–(1.3). Within this paper we investigate the most common case of the *total least squares problem* (TLS)

$$\min_{X,E,G} \|[G|E]\|_F \qquad \text{subject to} \qquad (A+E)X = B+G, \tag{1.4}$$

where $\|\cdot\|_F$ denotes the Frobenius norm.

The TLS problem with $d=1$ was for the first time analyzed in the paper [10] of Golub and Van Loan. This paper states the *sufficient condition* for existence of the TLS solution. The subsequent work of Van Huffel and Vandewalle [21] and the work of Wei [22], [23] follow essentially the path outlined in [10]. In particular, the theory is mostly based on the sufficient (not *necessary and sufficient*) condition for existence of the TLS solution. The core problem concept, introduced in [16] for $d=1$, is based on a different reasoning. It asks what does it mean in terms of the original data A and b that the solution in the TLS sense does not exist. Van Huffel and Vandewalle indicate that this happens in the presence of the so-called *unwanted colinearities*, when the linear dependency between the columns of A is stronger than the linear dependency between the range of A and the right-hand side b. The core problem reduction removes all redundancies or irrelevant information from the data $[b|A]$. Thus it allows to simply formulate the *necessary and sufficient condition* for the existence of the TLS solution for $d=1$; see [16]. Core problem can be obtained by the singular value decomposition (SVD) of A or by the Golub–Kahan iterative bidiagonalization [9]; see [16], [14].

The first steps in generalizing the core problem concept for the multiple right-hand side case $d>1$ were done by Björck in the series of talks [2], [3], [4], in the unpublished manuscript [5], by Sima in [19], by Sima and Van Huffel in [20], and by Plešinger in [18]. Following these works and the paper [11] fully classifying situations which can occur when $d>1$, the paper [13] provides a rigorous extension of the core problem concept to TLS with multiple right-hand sides (1.4). The orthogonal transformation (data reduction) used there is based on the SVD of the matrix A. The present paper investigates the *band generalization of the Golub–Kahan bidiagonalization* (or simply the *band algorithm*) with deflations, proposed in [2]–[5]. Here we prove that such approach indeed provides a core problem in the sense of [13]. Furthermore, this allows to derive additional properties of the core problem that might be useful in analysis of its solvability.

The paper is organized in the following way. Section 2 recalls the background results. Section 3 describes the band generalization of the Golub–Kahan bidiagonalization. Section 4 introduces generalized Jacobi matrices and analyzes properties of the band subproblem. Section 5 concludes the paper.

Throughout the text $\mathcal{R}(M)$ and $\mathcal{N}(M)$ denote the range and null-space of a matrix M, respectively; I_ℓ (or just I) denotes an $\ell\times\ell$ identity matrix; e_k denotes the kth column of I; $0_{\ell,\xi}$ (or just 0) denotes an $\ell\times\xi$ zero matrix; and $\|v\|$ denotes the Euclidean norm of a vector v. The following convention concerning the entries of matrices will simplify the exposition:

- club ($\clubsuit$) stands for a nonzero entry, $\clubsuit \neq 0$;
- heart ($\heartsuit$) stands for a general entry which can also be zero;
- empty spaces in matrices always represent zero entries.

Throughout the paper we assume *exact arithmetic*.

2. The core problem and other background results.

In order to make the text as self-consistent as possible, we briefly recall the known results used below.

2.1. Core problem. The *core problem* within the problem (1.1) is defined as follows (see [13, Definition 5.2]):

DEFINITION 2.1 (Core problem). *The subproblem $A_{11}X_1 \approx B_1$ is a core problem within the approximation problem $AX \approx B$ if $[B_1|A_{11}]$ is minimally dimensioned and A_{22} maximally dimensioned subject to the orthogonal transformations of the form*

$$P^T[B|A]\begin{bmatrix} R & 0 \\ 0 & Q \end{bmatrix} = P^T[BR|AQ] \equiv \left[\begin{array}{c|c||c|c} B_1 & 0 & A_{11} & 0 \\ \hline 0 & 0 & 0 & A_{22} \end{array}\right], \tag{2.1}$$

where $P^{-1} = P^T$, $Q^{-1} = Q^T$, $R^{-1} = R^T$.

Let $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ have k distinct singular values σ_j with multiplicities r_j and the orthonormal bases of the corresponding left singular vector subspaces $U_j \in \mathbb{R}^{\overline{m}\times r_j}$, $j = 1,\ldots,k$. Let $r_{k+1} \equiv \dim(\mathcal{N}(A_{11}^T))$, with $U_{k+1} \in \mathbb{R}^{\overline{m}\times r_{k+1}}$ having the orthonormal basis vectors of $\mathcal{N}(A_{11}^T)$ as its columns. Then $U \equiv [U_1,\ldots,U_k,U_{k+1}] \in \mathbb{R}^{\overline{m}\times\overline{m}}$ and $U^T = U^{-1}$. The core problem $A_{11}X_1 \approx B_1$ has the following properties (see [13, p. 925]):

(CP1) The matrix $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of *full column rank* equal to $\overline{n} \le \overline{m}$.

(CP2) The matrix $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$ is of *full column rank* equal to $\overline{d} \le \overline{m}$.

(CP3) The matrices $\Phi_j \equiv U_j^T B_1 \in \mathbb{R}^{r_j\times\overline{d}}$ are of *full row rank* equal to $r_j \le \overline{d}$, for $j = 1,\ldots,k+1$.

These properties guarantee minimality of the core problem; see [13, section 4]. Dimensions of any subproblem $A_{11}X_1 \approx B_1$ having the properties (CP1)–(CP3) cannot be reduced by any orthogonal transformation of the form (2.1). Moreover

$$U^T[B_1|A_{11}] = \left.\left[\begin{array}{c|c} \underbrace{\begin{array}{c}\Phi_1\\ \vdots\\ \Phi_k\\ \Phi_{k+1}\end{array}}_{\overline{d}} & \underbrace{\begin{array}{c}U_1^TA_{11}\\ \vdots\\ U_k^TA_{11}\\ 0\end{array}}_{\overline{n}}\end{array}\right]\begin{array}{l} \}r_1 \\ \vdots \\ \}r_k \\ \}r_{k+1}\end{array}\right\}\overline{m},$$

where $[U_1,\ldots,U_k]^TA_{11}$ is a square nonsingular matrix of the size $\overline{n}\times\overline{n}$, $\overline{n} = r_1+\ldots+r_k$, and Φ_{k+1} is of full row rank $r_{k+1} = \overline{m}-\overline{n}$. Thus (CP1)–(CP3) imply that the extended matrix $[B_1|A_{11}]$ is of *full row rank* equal to $\overline{m}$, $\max\{\overline{n},\overline{d}\} \le \overline{m} \le \overline{n}+\overline{d}$.

2.2. Golub–Kahan bidiagonalization. Consider first $d = 1$, i.e., the single right-hand side problem $Ax \approx b$. Here the core problem can be obtained by the *Golub–Kahan iterative bidiagonalization*[1]. Using the initial vectors $q_0 = 0$ and $p_1 = b/\gamma_1$, where $\gamma_1 = \|b\|$, it computes for $j = 1,2,\ldots$

$$q_j\alpha_j = A^Tp_j - q_{j-1}\gamma_j, \tag{2.2}$$
$$p_{j+1}\gamma_{j+1} = Aq_j - p_j\alpha_j, \tag{2.3}$$

such that $\|q_j\| = \|p_{j+1}\| = 1$, and $\alpha_j > 0$, $\gamma_{j+1} > 0$. The matrices

$$P_j \equiv [p_1,\ldots,p_j] \in \mathbb{R}^{m\times j}, \quad Q_j \equiv [q_1,\ldots,q_j] \in \mathbb{R}^{n\times j},$$

[1] Due to the close connection to the Lanczos algorithm one can also find it under the name the Golub–Kahan–Lanczos bidiagonalization; see, e.g., [1], [3], [4].

have orthonormal columns, $P_j^T P_j = Q_j^T Q_j = I_j$; see [9]. The iterative process (2.2)–(2.3) terminates when the right-hand side of one of the equations becomes zero, i.e., either $q_j \alpha_j = 0$ (in the incompatible case) or $p_{j+1}\gamma_{j+1} = 0$ (in the compatible case) for some j. Consider that $Ax \approx b$ is incompatible, $b \notin \mathcal{R}(A)$, and let $q_{\overline{n}+1}\alpha_{\overline{n}+1} = 0$. Then, denoting $P_1^{\rm cp} \equiv P_{\overline{n}+1}$ and $Q_1^{\rm cp} \equiv Q_{\overline{n}}$,

$$(P_1^{\rm cp})^T [b|AQ_1^{\rm cp}] = \left[\begin{array}{c|cccc} \gamma_1 & \alpha_1 & & & \\ & \gamma_2 & \ddots & & \\ & & \ddots & \alpha_{\overline{n}} & \\ & & & \gamma_{\overline{n}+1} & \end{array}\right] = [b_1|A_{11}] \in \mathbb{R}^{(\overline{n}+1)\times(\overline{n}+1)} \tag{2.4}$$

represents the core problem within $[b|A]$, and

$$P^T [b|A] \left[\begin{array}{cc} 1 & 0 \\ 0 & Q \end{array}\right] = \left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right], \qquad P \equiv [P_1^{\rm cp}, P_2^{\rm cp}], \qquad Q \equiv [Q_1^{\rm cp}, Q_2^{\rm cp}],$$

where $P_2^{\rm cp}$, $Q_2^{\rm cp}$ are chosen such that $P^{-1} = P^T$, $Q^{-1} = Q^T$; see [16]. A generalization of the Golub–Kahan bidiagonalization for the problems with multiple right-hand sides is given in section 3 below.

2.3. Right-hand side preprocessing. In order to get an equivalent problem with the full column rank right-hand sides matrix, we preprocess B in an analogous way as in [13, section 3.1]. Let $\overline{d} \equiv \operatorname{rank}(B) \leq \min\{m, d\}$, $B \in \mathbb{R}^{m\times d}$. Consider any decomposition of B in the form

$$B = [C, 0]R^T, \qquad C \in \mathbb{R}^{m\times\overline{d}}, \qquad R \in \mathbb{R}^{d\times d}, \tag{2.5}$$

where C is of *full column rank*, and R is square orthogonal, i.e. $R^{-1} = R^T$. Multiplication of (1.1) from the right by R gives

$$A(XR) \approx BR, \qquad \text{where} \qquad XR \equiv [Y, Y'] \in \mathbb{R}^{n\times d}, \qquad Y \in \mathbb{R}^{n\times\overline{d}} \tag{2.6}$$

(if $d = \overline{d}$, then it can be considered $R = I_d$, $B = C$, $X = Y$). The original problem (1.1) is in this way split into two subproblems,

$$AY \approx C \qquad \text{and} \qquad AY' \approx 0, \tag{2.7}$$

where the second problem is homogeneous. Following the arguments in [16], we consider the meaningful solution $Y' \equiv 0$. In this way, the approximation problem (1.1) reduces to $AY \approx C$ in (2.7). The full column rank matrix $C \in \mathbb{R}^{m\times\overline{d}}$ is called the *preprocessed right-hand side.*

Remark 2.2. A decomposition (2.5) can be obtained using the LQ decomposition of B (see [13, remark 3.1]) in the form

$$\Pi B = [\Lambda, 0]R^T, \qquad \Pi \in \mathbb{R}^{m\times m}, \quad \Lambda \in \mathbb{R}^{m\times\overline{d}}, \quad R \in \mathbb{R}^{d\times d},$$

where Π is a permutation matrix (representing possible row pivoting of B), and Λ is in a lower triangular column echelon form with nonzero columns. Then $C \equiv \Pi^T\Lambda$ is called the *LQ-preprocessed right-hand side.* Alternatively, one can use the SVD of B (see [13, section 3.1]) in the form

$$B = S[\Theta, 0]R^T, \qquad S \in \mathbb{R}^{m\times\overline{d}}, \quad \Theta \in \mathbb{R}^{\overline{d}\times\overline{d}}, \quad R \in \mathbb{R}^{d\times d}, \tag{2.8}$$

where S has mutually orthonormal columns, and the square nonsingular Θ contains the singular values of B on the diagonal. Then $C \equiv S\Theta$ has (nonzero) mutually orthogonal columns and it is called the *SVD-preprocessed right-hand side.*

3. Band generalization of the Golub–Kahan bidiagonalization. Now we describe in details the band algorithm. Consider the problem $AY \approx C$, where $C \in \mathbb{R}^{m\times\overline{d}}$ is of full column rank obtained above. As an extension of (2.4), we want to reduce $[C|A]$ to the upper triangular band matrix with (at most) $\overline{d}+1$ nonzero diagonals (all entries above the $\overline{d}$th superdiagonal are zero). We start with the QR decomposition of the right-hand side C. The basic band structure is then obtained using Householder reflections. The whole transformation can be reformulated as an iterative procedure that, employing deflations, reveals a subproblem representing the core problem analogously to (2.2)–(2.4).

3.1. Basic structure of the band algorithm. First, the right-hand side C is transformed to the upper triangular form. Consider the QR decomposition

$$C = P_{(0)}F, \qquad F = \begin{bmatrix} F_1 \\ 0 \end{bmatrix}, \qquad F_1 = \begin{bmatrix} \gamma_{1,1} & \beta_{1,2} & \cdots & \beta_{1,\overline{d}} \\ & \gamma_{2,2} & \ddots & \vdots \\ & & \ddots & \beta_{\overline{d}-1,\overline{d}} \\ & & & \gamma_{\overline{d},\overline{d}} \end{bmatrix}, \tag{3.1}$$

where $P_{(0)} \in \mathbb{R}^{m\times m}$, $P_{(0)}^{-1} = P_{(0)}^T$, and F_1 is the upper triangular square matrix with a positive diagonal, $\gamma_{j,j} > 0$, $j = 1,\ldots,\overline{d}$. If C is the *SVD-preprocessed right-hand side*, then $F_1 = \Theta$ is diagonal containing the singular values of the original right-hand side B, and the first $\overline{d}$ columns of $P_{(0)}$ are the columns of S; see (2.8). It should be noted that the matrix $P_{(0)}$ as well as the matrices $P_{(k)}$ below, which are all $\in \mathbb{R}^{m\times m}$, are distinct from the matrices $P_j \in \mathbb{R}^{m\times j}$ used above in description of the Golub–Kahan iterative bidiagonalization. Denote $L_{(0)} \equiv P_{(0)}^T A$, then

$$P_{(0)}^T[C|A] = [F|L_{(0)}]. \tag{3.2}$$

It remains to transform $L_{(0)}$ to a lower triangular band matrix with (at most) $\overline{d}+1$ nonzero diagonals (all entries below the $\overline{d}$th subdiagonal are zero). This can be done, e.g., by multiplications of $L_{(0)}$ with suitable Householder matrices $H_{Q,j}$, $H_{P,j}$, $j = 1,2,\ldots$ from the right and left, respectively. Let for $k = 1,2,\ldots$

$$P_{(k)} = P_{(0)}H_{P,1}H_{P,2}\ldots H_{P,k} \in \mathbb{R}^{m\times m}, \quad Q_{(k)} = H_{Q,1}H_{Q,2}\ldots H_{Q,k} \in \mathbb{R}^{n\times n} \tag{3.3}$$

be orthogonal matrices yielding a transformation

$$P_{(k)}^T[C|AQ_{(k)}] = [F|P_{(k)}^T AQ_{(k)}] \tag{3.4}$$

$$= \left[\begin{array}{cccc|cccccc} \gamma_{1,1} & \beta_{1,2} & \cdots & \beta_{1,\overline{d}} & \alpha_{1,\overline{d}+1} & & & & & \\ & \gamma_{2,2} & \ddots & \vdots & \beta_{2,\overline{d}+1} & \ddots & & & & \\ & & \ddots & \beta_{\overline{d}-1,\overline{d}} & \vdots & \ddots & \alpha_{k,\overline{d}+k} & & & \\ & & & \gamma_{\overline{d},\overline{d}} & \beta_{\overline{d},\overline{d}+1} & & \beta_{k+1,\overline{d}+k} & \heartsuit & \cdots & \heartsuit \\ & & & & \gamma_{\overline{d}+1,\overline{d}+1} & \ddots & \vdots & \vdots & & \vdots \\ & & & & & \ddots & \beta_{k+\overline{d}-1,\overline{d}+k} & \heartsuit & \cdots & \heartsuit \\ & & & & & & \gamma_{\overline{d}+k,\overline{d}+k} & \heartsuit & \cdots & \heartsuit \\ & & & & & & & \heartsuit & \cdots & \heartsuit \\ & & & & & & & \vdots & & \vdots \\ & & & & & & & \heartsuit & \cdots & \heartsuit \end{array}\right], \tag{3.5}$$

$$\text{with} \quad \alpha_{j,\overline{d}+j} > 0, \quad \gamma_{\overline{d}+j,\overline{d}+j} > 0, \quad \text{for} \quad j = 1, \ldots, k. \tag{3.6}$$

Denote

$$L_{(j)} \equiv P_{(j)}^T A Q_{(j)} = H_{P,j}^T L_{(j-1)} H_{Q,j}\,, \tag{3.7}$$

$$\text{and} \qquad L_{(j-)} \equiv P_{(j-1)}^T A Q_{(j)} = L_{(j-1)} H_{Q,j}\,, \qquad j = 1, \ldots, k. \tag{3.8}$$

The entry $\alpha_{j,\overline{d}+j}$ represents the norm of the trailing subrow (of length $n-j+1$) of the jth row of $L_{(j-1)}$, and analogously the entry $\gamma_{\overline{d}+j,\overline{d}+j}$ represents the norm of the trailing subcolumn (of length $m-j-\overline{d}+1$) of the jth column of $L_{(j-)}$. If the first row of $L_{(0)}$ is zero (i.e., $\alpha_{1,\overline{d}+1} = 0$), or if the trailing subcolumn of $L_{(1-)}$ of length $m-\overline{d}$ is zero (i.e., $\gamma_{\overline{d}+1,\overline{d}+1} = 0$), or if the problem does not have enough rows (i.e., $\gamma_{\overline{d}+1,\overline{d}+1}$ does not exist), then the transformation (3.4) to the form (3.5) with the condition (3.6) does not exist. In such case we formally put $k = 0$ and $Q_{(0)} \equiv I_n$. This particular case is discussed later in section 3.2. In the rest of this paragraph we for simplicity consider $\alpha_{j,\overline{d}+j} > 0$, $\gamma_{\overline{d}+j,\overline{d}+j} > 0$, $j = 1, \ldots, k$. Denote $p_1, \ldots, p_{\overline{d}+k}$ the first $\overline{d}+k$ columns of $P_{(k)}$ and $q_1, \ldots, q_k$ the first k columns of $Q_{(k)}$. Using (3.7) rewritten as

$$A Q_{(k)} = P_{(k)} L_{(k)} \qquad \text{and} \qquad A^T P_{(k)} = Q_{(k)} L_{(k)}^T, \tag{3.9}$$

we can write for Aq_j and $A^T p_j$

$$A q_j = [p_j, p_{j+1}, \ldots, p_{j+\overline{d}-1}, p_{j+\overline{d}}][\alpha_{j,\overline{d}+j}, \beta_{j+1,\overline{d}+j}, \ldots, \beta_{j+\overline{d}-1,\overline{d}+j}, \gamma_{\overline{d}+j,\overline{d}+j}]^T, \tag{3.10}$$

$$A^T p_j = [q_{j-\overline{d}}, q_{j-\overline{d}+1}, \ldots, q_{j-1}, q_j][\gamma_{j,j}, \beta_{j,j+1}, \ldots, \beta_{j,j+\overline{d}-1}, \alpha_{j,\overline{d}+j}]^T. \tag{3.11}$$

Using the initial vectors $p_1, \ldots, p_{\overline{d}}$ given by (3.1) and $q_{1-\overline{d}} = \ldots = q_0 \equiv 0$, the columns of the $(\overline{d}+k) \times k$ leading principal block of $L_{(k)}$, and the columns $q_1, \ldots, q_k$, and $p_{\overline{d}+1}, \ldots, p_{\overline{d}+k}$ are iteratively generated by

$$q_j \alpha_{j,\overline{d}+j} \equiv A^T p_j - q_{j-\overline{d}} \gamma_{j,j} - \left(\sum_{i=1}^{\overline{d}-1} q_{j-\overline{d}+i} \beta_{j,j+i} \right), \tag{3.12}$$

$$\beta_{j+i,\overline{d}+j} \equiv p_{j+i}^T A q_j, \qquad \text{for} \quad i = 1, \ldots, \overline{d}-1, \tag{3.13}$$

$$p_{\overline{d}+j} \gamma_{\overline{d}+j,\overline{d}+j} \equiv A q_j - p_j \alpha_{j,\overline{d}+j} - \left(\sum_{i=1}^{\overline{d}-1} p_{j+i} \beta_{j+i,\overline{d}+j} \right), \tag{3.14}$$

where $\|q_j\| = \|p_{j+\overline{d}}\| = 1$, $\alpha_{j,\overline{d}+j} > 0$, $\gamma_{\overline{d}+j,\overline{d}+j} > 0$, for $j = 1, 2, \ldots, k$. The β entries represent orthogonalization coefficients.

3.2. Deflation in the band algorithm. Now we focus on the case when the right-hand side of (3.12) or (3.14) becomes zero (including the case $k = 0$). Let ℓ be the *first* index for which *either* $q_\ell \alpha_{\ell,\overline{d}+\ell} = 0$ (yielding formally $\alpha_{\ell,\overline{d}+\ell} = 0$), *or* $p_{\overline{d}+\ell} \gamma_{\overline{d}+\ell,\overline{d}+\ell} = 0$ (yielding formally $\gamma_{\overline{d}+\ell,\overline{d}+\ell} = 0$), $1 \leq \ell \leq \min\{n+1, m-\overline{d}+1\}$. The cases $\ell = n+1$ and $\ell = m-\overline{d}+1$ represent reaching the number of columns and rows of the system matrix, respectively.

3.2.1. Upper deflation. Let for $\ell < n+1$ we get $q_\ell \alpha_{\ell,\overline{d}+\ell} = 0$. Recall that $\alpha_{\ell,\overline{d}+\ell}$ is the norm of a trailing subrow of the ℓth row of $L_{(\ell-1)} = P_{(\ell-1)}^T A Q_{(\ell-1)}$ to the right of $\beta_{\ell,\overline{d}+\ell-1}$, therefore

$$P_{(\ell-1)}^T[C|AQ_{(\ell-1)}] = [F|L_{(\ell-1)}] = \begin{bmatrix} \ddots & & & & \\ \ddots & \alpha_{\ell-1,\overline{d}+\ell-1} & & & \\ \ddots & \beta_{\ell,\overline{d}+\ell-1} & 0 & \cdots & 0 \\ & \beta_{\ell+1,\overline{d}+\ell-1} & \heartsuit & \cdots & \heartsuit \\ & \vdots & \vdots & & \vdots \end{bmatrix}. \tag{3.15}$$

In this case the Householder matrix $H_{Q,\ell}$ is constructed to transform the first row below the ℓth row having a nonzero trailing subrow (say, the ξth row) while producing $\alpha_{\xi,\overline{d}+\ell} > 0$.

This *upper deflation* can be easily described using (3.12)–(3.14). Consider that the $(\ell+1)$th row of $[F|L_{(\ell-1)}]$ has the nonzero trailing subrow. The formula for computing $\alpha_{\ell+1,\overline{d}+\ell} > 0$ and q_ℓ is then given by equating the $(\ell+1)$th (instead of the ℓth) columns of $A^T P_{(\ell)} = Q_{(\ell)} L_{(\ell)}^T$; see also (3.9) and (3.11). Formulas (3.12)–(3.14) are then for $j = \ell, \ell+1, \ldots$, modified to

$$\begin{aligned} q_j \alpha_{j+1,\overline{d}+j} &\equiv A^T p_{j+1} - q_{j-\overline{d}+1}\gamma_{j+1,j+1} - \left(\sum\nolimits_{i=2}^{\overline{d}-1} q_{j-\overline{d}+i}\beta_{j+1,j+i}\right), && (3.16)\\ \beta_{j+i,\overline{d}+j} &\equiv p_{j+i}^T A q_j, \qquad \text{for} \quad i = 2,\ldots,\overline{d}-1, && (3.17)\\ p_{\overline{d}+j}\gamma_{\overline{d}+j,\overline{d}+j} &\equiv A q_j - p_{j+1}\alpha_{j+1,\overline{d}+j} - \left(\sum\nolimits_{i=2}^{\overline{d}-1} p_{j+i}\beta_{j+i,\overline{d}+j}\right). && (3.18) \end{aligned}$$

The *number of summands* and *computed coefficients* β is *reduced by one* for all $j \geq \ell$. Each upper deflation changes the pattern of nonzero entries in the band matrix by reducing the *effective bandwidth* from the top by one.

3.2.2. Lower deflation. Let for $\ell < m - \overline{d} + 1$ we get $p_{\overline{d}+\ell}\gamma_{\overline{d}+\ell,\overline{d}+\ell} = 0$. Recall that $\gamma_{\overline{d}+\ell,\overline{d}+\ell}$ is the norm of a trailing subcolumn of the ℓth column of $L_{(\ell-)} = P_{(\ell-1)}^T AQ_{(\ell)}$ below $\beta_{\ell+\overline{d}-1,\overline{d}+\ell}$, therefore

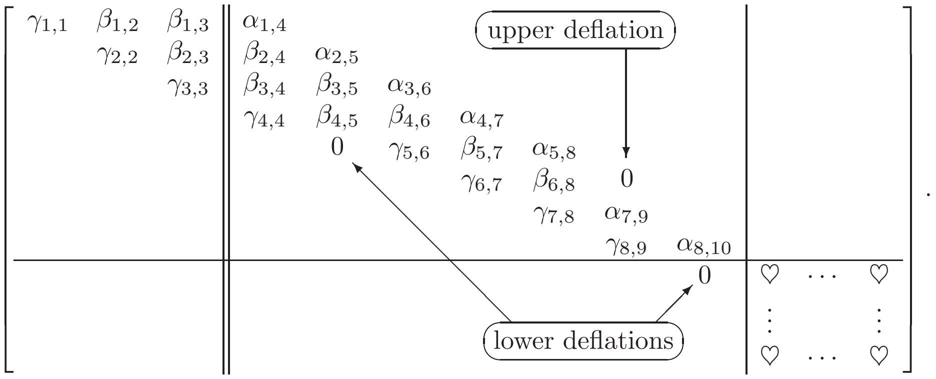
$$P_{(\ell-1)}^T[C|AQ_{(\ell)}] = [F|L_{(\ell-)}] = \begin{bmatrix} \ddots & \ddots & \vdots & \vdots & \\ & \gamma_{\overline{d}+\ell-1,\overline{d}+\ell-1} & \beta_{\ell+\overline{d}-1,\overline{d}+\ell} & \heartsuit & \cdots \\ & & 0 & \heartsuit & \cdots \\ & & \vdots & \vdots & \\ & & 0 & \heartsuit & \cdots \end{bmatrix}. \tag{3.19}$$

Then we take $H_{P,\ell} = I_m$. The matrix $L_{(\ell-)}$ in (3.19) is multiplied by $H_{Q,\ell+1}$ from the right, giving $\alpha_{\ell+1,\overline{d}+\ell+1}$, and the algorithm proceeds with transformation of the $(\ell+1)$th column (provided its trailing subcolumn is nonzero). For capturing this *lower deflation* analogously as above, it is convenient to consider a row-oriented formulation of (3.12)–(3.14). Each lower deflation modifies the pattern of nonzero entries in the band matrix by reducing the effective bandwidth from the bottom by one.

3.2.3. Band subproblem. Since the matrix $[F|L_{(k)}]$ has $(\overline{d}+1)$ nonzero diagonals (see (3.5)), after $\overline{d}$ deflations the effective bandwidth is reduced to one. Denote $P \in \mathbb{R}^{m\times m}$, $Q \in \mathbb{R}^{n\times n}$ the products of the resulting Householder matrices (see (3.3)) and denote $L \equiv P^T AQ$. Then

$$P^T[C|AQ] = [F|L] \equiv \left[\begin{array}{c||c|c} B_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array}\right] \tag{3.20}$$

and the problem is decomposed in the desired subproblems, see, e.g., the following illustration:



Let $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$, $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$, and denote $P_1^{\mathrm{cp}} \equiv [p_1, \ldots, p_{\overline{m}}] \in \mathbb{R}^{m\times\overline{m}}$, $Q_1^{\mathrm{cp}} \equiv [q_1, \ldots, q_{\overline{n}}] \in \mathbb{R}^{n\times\overline{n}}$. In the rest of this paper we show that the *band subproblem*

$$(P_1^{\mathrm{cp}})^T[C|AQ_1^{\mathrm{cp}}] = [B_1|A_{11}] \in \mathbb{R}^{\overline{m}\times(\overline{n}+\overline{d})} \tag{3.21}$$

represents the core problem, by proving that it satisfies the properties (CP1)–(CP3); see section 2.1.

An implementation of the band algorithm with inputs A and B, and outputs A_{11}, B_1, P_1^{cp}, Q_1^{cp}, and R (see (2.5)) can be found in Appendix A. For alternative implementations see [19, Algorithm 2.4, p. 38] or [18, Algorithm 5.1, p. 74].

4. Core problem in the band form. The equations (3.20)–(3.21) immediately give

$$A^T P_1^{\mathrm{cp}} = Q \left[\begin{array}{c} A_{11}^T \\ \hline 0 \end{array}\right], \qquad \text{and} \qquad [C|AQ_1^{\mathrm{cp}}] = P \left[\begin{array}{c|c} B_1 & A_{11} \\ \hline 0 & 0 \end{array}\right],$$

which represent QR decompositions of matrices $A^T P_1^{\mathrm{cp}}$ and $[C|AQ_1^{\mathrm{cp}}]$, respectively. The matrix A_{11} is in the lower triangular column echelon form with nonzero columns, thus it is of *full column rank* $\overline{n}$ giving the property (CP1). The right-hand side B_1 is in the upper triangular form with nonzero entries on the diagonal (see (3.1)), thus it is of *full column rank* $\overline{d}$ giving the property (CP2). Further $[B_1|A_{11}]$ is in the upper triangular row echelon form with nonzero rows, thus it is of *full row rank* $\overline{m}$ giving the inequality

$$\max\{\overline{n}, \overline{d}\} \leq \overline{m} \leq \overline{n} + \overline{d}. \tag{4.1}$$

Note that for $\overline{d} = 1$ the matrix B_1 becomes a vector b_1, the band algorithm becomes the standard Golub–Kahan bidiagonalization of A, the matrices $[b_1|A_{11}]$, A_{11} become bidiagonal with $[b_1|A_{11}]^T[b_1|A_{11}]$, $A_{11}A_{11}^T$, and $A_{11}^T A_{11}$, representing Jacobi matrices (symmetric tridiagonal matrices with positive subdiagonal entries). This relationship has been used in [14] and [12]. Jacobi matrices represent thoroughly studied objects with the origin in the first half of the 19th century; see the historical note 3.4.3 in [15, section 3.4, pp. 108–136]; see also [17, Chapter 7, pp. 119–150], [24, section 5, §36–§48, pp. 299–316], and [7, Chapter 1.3, pp. 10–20].

In the following we introduce generalized Jacobi matrices, discuss their spectral properties, and show their relationship to the band subproblem with $\overline{d} > 1$. In particular, we investigate bases of eigenspaces of generalized Jacobi matrices in section 4.1, and we show that $A_{11}A_{11}^T$ represents generalized Jacobi matrix in section 4.2. As a consequence, the bases of the left singular vector subspaces of A_{11} have the properties guaranteeing that the band subproblem $[B_1|A_{11}]$ satisfies also the property (CP3). Other generalizations of Jacobi matrices can be found, e.g., in [6, Chapter 3].

4.1. Generalized Jacobi matrices. Let $T \in \mathbb{R}^{n\times n}$ be a symmetric matrix with entries $t_{k,j}$. In analogy to the notation in, e.g., [8, section 4.1], we consider for $k = 1, \ldots, n$

$$f(k) = \min\{j \,:\, t_{k,j} \neq 0\}, \qquad \text{and} \qquad h(k) = k - f(k). \tag{4.2}$$

The number $f(k)$ is the column index of the first nonzero entry in the kth row of T (provided it exists), and $h(k)$ is the distance between this and the diagonal entry. Consider the following matrices.

Definition 4.1 (ρ-wedge-shaped matrix). *Let $T \in \mathbb{R}^{n\times n}$ be a symmetric matrix, and ρ, $1 \leq \rho < n$, an integer. If $h(k)$ for $k = \rho+1, \ldots, n$ is positive and nonincreasing, then we call T a ρ-wedge-shaped matrix.*

For clarity we give some examples of 3-wedge-shaped matrices:

$$\begin{bmatrix} \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & \\ \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit \\ & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit \\ & & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit \\ & & & \clubsuit & \heartsuit & \heartsuit & \heartsuit \end{bmatrix}, \begin{bmatrix} \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & & & \\ \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & \\ \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & \\ & & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \\ & & & \clubsuit & \heartsuit & \heartsuit & \clubsuit \\ & & & & & \clubsuit & \heartsuit \end{bmatrix}, \begin{bmatrix} \heartsuit & \heartsuit & \heartsuit & & & & \\ \heartsuit & \heartsuit & \heartsuit & & & & \\ \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\ & & \clubsuit & \heartsuit & \clubsuit & & \\ & & & \clubsuit & \heartsuit & \clubsuit & \\ & & & & \clubsuit & \heartsuit & \clubsuit \\ & & & & & \clubsuit & \heartsuit \end{bmatrix}.$$

Recall that clubs ($\clubsuit$) stand for nonzero entries, and hearts ($\heartsuit$) stand for general entries which can also be zero. Since 1-wedge-shaped matrices are symmetric tridiagonal with nonzero subdiagonal entries, the wedge-shaped matrices can be seen as a generalization of Jacobi matrices.

Jacobi matrices have simple eigenvalues; see, e.g., [17, Lemma 7.7.1]. In the text below it is shown that multiplicities of eigenvalues of a ρ-wedge-shaped matrix are bounded by ρ. The following example of a 2-wedge-shaped matrix

$$\begin{bmatrix} 0 & 0 & 1 & & \\ 0 & 0 & 0 & \ddots & \\ 1 & 0 & 0 & \ddots & 1 \\ & \ddots & \ddots & \ddots & 0 \\ & & 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & & \\ 1 & 0 & 1 & \\ & 1 & 0 & 1 \\ & & 1 & 0 \end{bmatrix} \otimes I_2 \in \mathbb{R}^{8\times 8}$$

with eigenvalues

$$\lambda_{1,2} = -\frac{\sqrt{5}+1}{2}, \quad \lambda_{3,4} = -\frac{\sqrt{5}-1}{2}, \quad \lambda_{5,6} = \frac{\sqrt{5}-1}{2}, \quad \lambda_{7,8} = \frac{\sqrt{5}+1}{2}$$

illustrates that the bound is sharp, in the sense that the multiple eigenvalues with the multiplicity ρ can be present. This also shows that the *strict interlacing property* of eigenvalues of Jacobi matrices (see, e.g., [17, section 7.10]) does not hold for wedge-shaped matrices. Eigenvectors of Jacobi matrices have nonzero first and last entries; see, e.g., [17, Theorem 7.9.3 (7.9.5 in the original Prentice-Hall edition)]. The following theorem shows how to generalize the property of the nonzero first element to leading subvectors of eigenvectors of wedge-shaped matrices. This immediately gives the bound for the multiplicities of the individual eigenvalues. Subsequently we show how to generalize the property of the nonzero last element to eigenvectors of wedge-shaped matrices.

THEOREM 4.2. *Let $T \in \mathbb{R}^{n\times n}$ be a ρ-wedge-shaped matrix, $1 \le \rho < n$. Let $\lambda \in \mathbb{R}$, $v = [\nu_1, \ldots, \nu_n]^T \in \mathbb{R}^n$ be an eigenpair of T, i.e., $Tv = \lambda v$, $v \ne 0$. Then the leading subvector $[\nu_1, \ldots, \nu_\rho]^T \in \mathbb{R}^\rho$ of v is nonzero.*

Proof. Because $h(k)$, $k = \rho+1, \ldots, n$ is nonincreasing, the first nonzero entry $t_{k,f(k)}$ in the kth row is also the last nonzero entry in the $(f(k))$th column of T. Using the symmetry of T, $t_{f(k),k}$ is the last nonzero entry in the $(f(k))$th row. Thus the $(f(k))$th row of $Tv = \lambda v$ can for $k = \rho+1, \ldots, n$ be written as

$$\left(\sum_{\ell=1}^{k-1} t_{f(k),\ell}\,\nu_\ell\right) + t_{f(k),k}\,\nu_k = \lambda\,\nu_{f(k)}. \tag{4.3}$$

Let, by contradiction, $\nu_1 = \ldots = \nu_\rho = 0$. Then (4.3) is for $k = \rho+1$ reduced to

$$t_{f(\rho+1),\rho+1}\,\nu_{\rho+1} = \lambda\,\nu_{f(\rho+1)}.$$

Because $h(\rho+1)$ is positive, $f(\rho+1) < \rho+1$, and $\nu_{f(\rho+1)} = 0$. Since $t_{f(\rho+1),\rho+1} \ne 0$, then $\nu_{\rho+1} = 0$. Repeating the argument gives for $k = \rho+2, \ldots, n$, $\nu_{\rho+2} = \ldots = \nu_n = 0$, which contradicts $v \ne 0$. □

This theorem has the following corollary.

COROLLARY 4.3. *Let $T \in \mathbb{R}^{n\times n}$ be a ρ-wedge-shaped matrix, $1 \le \rho < n$. Let $\lambda \in \mathbb{R}$ be an eigenvalue of T with the multiplicity r. Let $v_\ell = [\nu_{1,\ell}, \ldots, \nu_{n,\ell}]^T \in \mathbb{R}^n$, $\ell = 1, \ldots, r$, be an arbitrary basis of the corresponding eigenspace, i.e., $TV = \lambda V$, where $V \equiv [v_1, \ldots, v_r] \in \mathbb{R}^{n\times r}$. Then the leading $\rho \times r$ block of V,*

$$\Omega \equiv \begin{bmatrix} \nu_{1,1} & \cdots & \nu_{1,r} \\ \vdots & \ddots & \vdots \\ \nu_{\rho,1} & \cdots & \nu_{\rho,r} \end{bmatrix} \in \mathbb{R}^{\rho\times r}, \tag{4.4}$$

is of full column rank r.

Proof. Since $Vw = [\omega_1, \ldots, \omega_n]^T$ represents for any $w \ne 0 \in \mathbb{R}^r$ an eigenvector of T, by theorem 4.2, $\Omega w = [\omega_1, \ldots, \omega_\rho]^T$ is nonzero, which gives the assertion. □

If $r > \rho$, then there exists a nontrivial linear combination of the columns of V which gives a vector with the first ρ entries zero, i.e., $\Omega \in \mathbb{R}^{\rho\times r}$ can obviously not have full column rank. This gives the bound for the multiplicities of individual eigenvalues:

COROLLARY 4.4. *An eigenvalue of a ρ-wedge-shaped matrix $T \in \mathbb{R}^{n\times n}$, $1 \le \rho < n$, has multiplicity at most ρ.*

The following theorem generalizes the property of the last nonzero element of eigenvectors of Jacobi matrices to eigenvectors of wedge-shaped matrices. The proof is analogous to the proof of theorem 4.2.

THEOREM 4.5. *Let $T \in \mathbb{R}^{n\times n}$ be a ρ-wedge-shaped matrix, $1 \leq \rho < n$. Let $\lambda \in \mathbb{R}$, $v = [\nu_1, \ldots, \nu_n]^T \in \mathbb{R}^n$ be an eigenpair of T, i.e., $Tv = \lambda v$, $v \neq 0$. Denote*

$$\{s_1, \ldots, s_\rho\} \equiv \{1, \ldots, n\} \setminus \{f(k) \,:\, k = \rho+1, \ldots, n\},$$
$$s_1 < s_2 < \ldots < s_\rho\,,$$

where $f(k)$ is given by (4.2). Then the subvector $[\nu_{s_1}, \ldots, \nu_{s_\rho}]^T \in \mathbb{R}^\rho$ of v is nonzero.

Proof. Since $t_{k,f(k)}$ is the first nonzero entry in the kth row of T, the kth row of $Tv = \lambda v$ can for $k = \rho+1, \ldots, n$ be written as

$$t_{k,f(k)}\,\nu_{f(k)} + \left(\sum\nolimits_{\ell=f(k)+1}^{n} t_{k,\ell}\,\nu_\ell\right) = \lambda\,\nu_k. \tag{4.5}$$

Let, by contradiction, $\nu_{s_1} = \ldots = \nu_{s_\rho} = 0$. Because $h(n)$ is positive, $f(n) < n$, and $\nu_\ell = 0$ for all $\ell > f(n)$, in particular, $\nu_n \equiv \nu_{s_\rho} = 0$. Thus (4.5) is for $k = n$ reduced to

$$t_{n,f(n)}\,\nu_{f(n)} = 0,$$

and $t_{n,f(n)} \neq 0$ gives $\nu_{f(n)} = 0$. Repeating the argument for $k = n-1, n-2, \ldots$ up to $\rho+1$ gives $\nu_{f(n-1)} = \nu_{f(n-2)} = \ldots = \nu_{f(\rho+1)} = 0$, which contradicts $v \neq 0$. □

Note that $s_1, \ldots, s_\rho$ represent the row (and column) indices where the effective bandwidth of T is reduced by one, and $s_\rho = n$. Both nonzero subvectors of length ρ described by theorems 4.2 and 4.5 can be observed from the pattern of a wedge-shaped matrix. As an illustration, eigenvectors of the following 3-wedge-shaped matrix of the size 9 have nonzero subvectors $[\nu_1, \nu_2, \nu_3]^T$ and $[\nu_3, \nu_6, \nu_9]^T$:

$$\begin{bmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \\ \nu_4 \\ \nu_5 \\ \nu_6 \\ \nu_7 \\ \nu_8 \\ \nu_9 \end{bmatrix}
\begin{array}{c} \longleftrightarrow \\ \longleftrightarrow \\ \longleftrightarrow \\ \\ \\ \\ \\ \\ \\ \end{array}
\begin{bmatrix}
\heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & & \\
\heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & & \\
\heartsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & & & & \\
\clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & & \\
 & \clubsuit & \heartsuit & \heartsuit & \heartsuit & \heartsuit & \clubsuit & & \\
 & & & \clubsuit & \heartsuit & \heartsuit & \heartsuit & & \\
 & & & & \clubsuit & \heartsuit & \heartsuit & \clubsuit & \\
 & & & & & & \clubsuit & \heartsuit & \clubsuit \\
 & & & & & & & \clubsuit & \heartsuit
\end{bmatrix}
\begin{array}{c} \\ \\ \longleftrightarrow \\ \\ \\ \longleftrightarrow \\ \\ \\ \longleftrightarrow \end{array}
\begin{bmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \\ \nu_4 \\ \nu_5 \\ \nu_6 \\ \nu_7 \\ \nu_8 \\ \nu_9 \end{bmatrix}.$$

4.2. Singular values and vectors of the band subproblem. To prove (CP3), we first show the link of the band subproblem (3.20)–(3.21) to the wedge-shaped matrices. For a positive definite matrix $M = Z^TZ$ with its (upper triangular) Cholesky factor Z it is well known that

$$\mathrm{env}(M) = \mathrm{env}(Z^T + Z), \qquad \text{where} \qquad \mathrm{env}(T) = \{(k,j) \,:\, f(k) \leq j < k\} \tag{4.6}$$

denotes the so-called *envelope* of a symmetric matrix T, and $f(k)$ is given by (4.2); see, e.g., [8, section 4.2]. Analogously, using the structure of the band subproblem (3.20)–(3.21), it is reasonable to expect that the symmetric positive semidefinite matrices $A_{11}A_{11}^T$ and $[B_1|A_{11}]^T[B_1|A_{11}]$ inherit the band structure and represent wedge-shaped matrices. However, their full row rank upper triangular factors A_{11}^T and $[B_1|A_{11}]$, respectively, do not represent the Cholesky factors, in general. Thus the above mentioned result cannot be used directly; see also an example in Figure 4.1. Therefore we

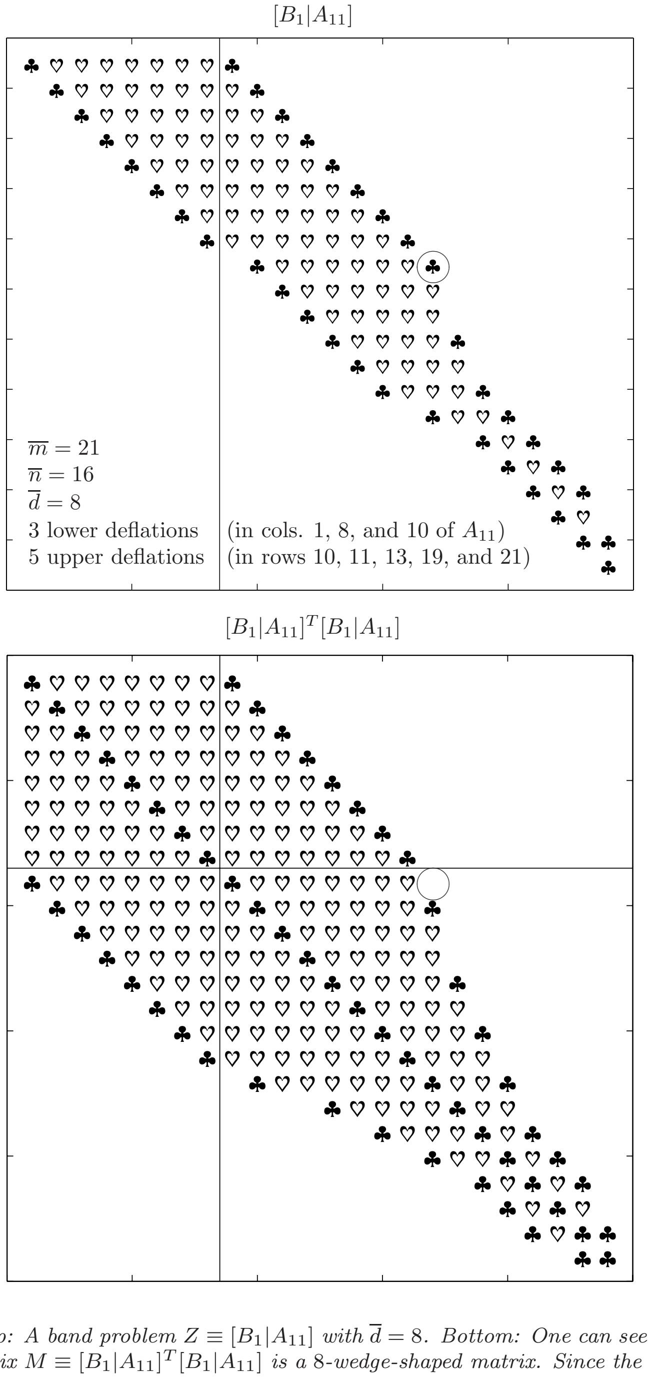


FIG. 4.1. *Top: A band problem* $Z \equiv [B_1|A_{11}]$ *with* $\overline{d} = 8$. *Bottom: One can see that the positive semidefinite matrix* $M \equiv [B_1|A_{11}]^T[B_1|A_{11}]$ *is a* 8*-wedge-shaped matrix. Since the upper triangular matrix* Z *in the top does not represent the Cholesky factor of the matrix* M *in the bottom, then* $\mathrm{env}(M) \neq \mathrm{env}(Z^T + Z)$; *see, e.g., the encircled nonzero entry in the top part and the encircled zero entry in the bottom part.*

state and prove the following lemma which shows when $A_{11}A_{11}^T$ and $[B_1|A_{11}]^T[B_1|A_{11}]$ are wedge-shaped matrices.

Lemma 4.6. *Let $A_{11}X_1 \approx B_1$, $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$, $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$ be the band subproblem (3.20)–(3.21). If $\overline{m} > \overline{d}$, then the matrix*

$$A_{11}A_{11}^T \in \mathbb{R}^{\overline{m}\times\overline{m}},$$

is $\overline{d}$-wedge-shaped. Since $\overline{d}+\overline{n} > \overline{d}$, then the matrix

$$[B_1|A_{11}]^T[B_1|A_{11}] \in \mathbb{R}^{(\overline{d}+\overline{n})\times(\overline{d}+\overline{n})},$$

is also $\overline{d}$-wedge-shaped.

Proof. Denote $a_k^T \equiv e_k^T A_{11}$ the kth *row* of A_{11}, thus $a_k^T a_j$ represents the (k,j)th entry of $A_{11}A_{11}^T$. We look for the first nonzero entry in the kth row of $A_{11}A_{11}^T$, $k = \overline{d}+1,\dots,\overline{m}$. Denote $\varphi(j) \in \{1,\dots,\overline{m}\}$ the row index of the first nonzero entry in the jth column of A_{11}, i.e.,

$$a_{\varphi(j)}^T = [\underbrace{\heartsuit,\dots,\heartsuit}_{j-1}, \alpha_{\varphi(j),\overline{d}+j}, \underbrace{0,\dots,0}_{\overline{n}-j}], \qquad j = 1,\dots,\overline{n}. \tag{4.7}$$

Denote $\psi(k) \in \{1,\dots,\overline{n}\}$ the column index of the first nonzero entry in the kth row of A_{11}, i.e.,

$$a_k^T = [\underbrace{0,\dots,0}_{\psi(k)-1}, \gamma_{k,\overline{d}+\psi(k)}, \underbrace{\heartsuit,\dots,\heartsuit}_{\overline{n}-\psi(k)}], \qquad k = \overline{d}+1,\dots,\overline{m}. \tag{4.8}$$

For $j = \psi(k)$ the entries $\alpha_{\varphi(j),\overline{d}+j}$ and $\gamma_{k,\overline{d}+\psi(k)}$ belong to the same column, i.e.,

$$a_k^T a_{\varphi(\psi(k))} = \gamma_{k,\overline{d}+\psi(k)}\, \alpha_{\varphi(\psi(k)),\overline{d}+\psi(k)} > 0. \tag{4.9}$$

Using the lower echelon form of A_{11}, all rows above $a_{\varphi(\psi(k))}^T$ ((4.7) with $j = \psi(k)$) are *structurally orthogonal* to a_k^T (4.8), thus all entries to the left of $a_k^T a_{\varphi(\psi(k))}$ (4.9) are zero. Consequently, $a_k^T a_{\varphi(\psi(k))}$ (4.9) is the *first nonzero entry* in the kth row of $A_{11}A_{11}^T$, $k = \overline{d}+1,\dots,\overline{m}$. Thus

$$f(k) = \varphi(\psi(k)),$$

see (4.2). The matrix A_{11} has the band form with the α entries located on the top and the γ entries on the bottom of the band; see section 3.2.3 above. The row $a_{\varphi(\psi(k))}^T$ ((4.7) with $j = \psi(k)$) is always placed above the row (4.8). Thus (4.9) is on the left of the diagonal entry $a_k^T a_k$ in the kth row of $A_{11}A_{11}^T$, i.e., $\varphi(\psi(k)) < k$ and

$$h(k) = k - \varphi(\psi(k))$$

is positive for $k = \overline{d}+1,\dots,\overline{m}$. Because both $\varphi(j)$ and $\psi(k)$ are increasing, the composed function $\varphi(\psi(k))$ is also increasing, and $h(k)$ is nonincreasing for $k = \overline{d}+1, \dots,\overline{m}$. Consequently, $A_{11}A_{11}^T$ is a $\overline{d}$-wedge-shaped-matrix.

The proof for $[B_1|A_{11}]^T[B_1|A_{11}]$ is analogous: Replace A_{11} by $[B_1|A_{11}]^T$ and exchange the roles of the α and γ entries. □

Recall that $\overline{m} \geq \max\{\overline{n},\overline{d}\}$; see (4.1). Thus the only case not covered by the previous lemma is $\overline{m} = \overline{d}$, where $A_{11}A_{11}^T$ has no particular structure. Note that $\overline{d}+\overline{n} =$

$\overline{d}$ (i.e., A_{11} has no columns) occurs in the excluded case $A^T B = 0$ (after the QR decomposition (3.1)–(3.2), the band algorithm starts with $\overline{d}$ upper deflations). The matrix $A_{11}^T A_{11} \in \mathbb{R}^{\overline{n}\times\overline{n}}$ is the trailing principal block of the $\overline{d}$-wedge-shaped matrix $[B_1|A_{11}]^T[B_1|A_{11}]$. If $\overline{n} > \overline{d}$, then $A_{11}^T A_{11}$ represents a $\overline{d}$-wedge-shaped matrix; see also Figure 4.1. If $\overline{n} \leq \overline{d}$, then $A_{11}^T A_{11}$ has no particular structure.

Now we are ready to apply the spectral properties of wedge-shaped matrices proved in section 4.1 to the band subproblem (3.20)–(3.21).

COROLLARY 4.7. *Let $A_{11}X_1 \approx B_1$, $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$, $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$ be the band subproblem* (3.20)–(3.21)*, i.e., $[B_1|A_{11}]$ and A_{11} are the upper and lower triangular band matrices, respectively, with (at most) $\overline{d}+1$ nonzero diagonals. Then:*

(a) *The singular values of $[B_1|A_{11}]$ and A_{11} have multiplicities at most $\overline{d}$.*

(b) *Let $v_1, \ldots, v_r$ be an orthonormal basis of the right singular vector subspace of $[B_1|A_{11}]$ corresponding to a singular value with the multiplicity r (or of the null-space $\mathcal{N}([B_1|A_{11}])$ with the dimension r). Then the leading $\overline{d}\times r$ block of $[v_1, \ldots, v_r] \in \mathbb{R}^{(\overline{n}+\overline{d})\times r}$ is of full column rank r.*

(c) *Let $u_1, \ldots, u_r$ be an orthonormal basis of the left singular vector subspace of A_{11} corresponding to a singular value with the multiplicity r (or of the null-space $\mathcal{N}(A_{11}^T)$ with the dimension r). Then the matrix*

$$\Phi \equiv [u_1, \ldots, u_r]^T B_1 \in \mathbb{R}^{r\times\overline{d}}$$

is of full row rank r, i.e., the band subproblem $A_{11}X_1 \approx B_1$ satisfies the condition (CP3)*; see section 2.1.*

Proof. Assertion (a) follows directly from lemma 4.6 and corollary 4.4, except for the case of A_{11} with $\overline{m} = \overline{d}$. Since $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$ is of full column rank, $\overline{m} \geq \overline{n}$, the assertion becomes in this case trivial. Assertion (b) follows directly from lemma 4.6 and corollary 4.3. Assertion (c): The leading block $\Omega \in \mathbb{R}^{\overline{d}\times r}$ of $[u_1, \ldots, u_r] \in \mathbb{R}^{\overline{m}\times r}$, is of full column rank r by corollary 4.3 (the case $\overline{m} = \overline{d}$ excluded in lemma 4.6 becomes again trivial) and $B_1 = [F_1^T, 0]^T$, where $F_1 \in \mathbb{R}^{\overline{d}\times\overline{d}}$ is nonsingular; see (3.1). Thus Φ is of full row rank r. ☐

Consequently, we have proved that the band algorithm computes the problem $A_{11}X_1 \approx B_1$ that satisfies conditions (CP1)–(CP3) defining the core problem formulated in section 2.1. We state this result as the following theorem.

THEOREM 4.8. *The band subproblem $A_{11}X_1 \approx B_1$* (3.20)–(3.21) *obtained as the output of the band algorithm described in section 3 applied on the problem $AX \approx B$ represents a core problem within $AX \approx B$ in the sense of definition 2.1. It can therefore be called the core problem in the band form.*

5. Concluding remarks.

We have shown that the band generalization of the Golub–Kahan iterative bidiagonalization algorithm always yields the minimally dimensioned subproblem within the original linear approximation problem $AX \approx B$. This consistently extends the results obtained in [16] to problems with multiple right-hand sides.

Assertions (a) and (b) of corollary 4.7 give some additional properties of core problems. For $\overline{d} = 1$, these properties reduce to the well known facts that singular values of $[b_1|A_{11}]$ are simple and the right singular vectors have nonzero first components, guaranteeing existence of the unique TLS solution of the core problem. The properties from corollary 4.7 might be helpful in analysis of solvability of core problems for $\overline{d} > 1$. This issue is, however, still under investigation.

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Appendix A. Implementation of the band algorithm.

Algorithm 1 implements the band algorithm. Assuming exact arithmetic, it returns for general input data A, B the matrices A_{11}, B_1 of the core problem in the band form, and the corresponding transformation matrices P_1^{cp}, Q_1^{cp} (see (3.21)), and R (see (2.5)). For alternative implementations see [19, Algorithm 2.4, p. 38] or [18, Algorithm 5.1, p. 74]. In the algorithm p_k, q_j denote the kth and jth column of P and Q, and $P_k \equiv [p_1, \ldots, p_k] \in \mathbb{R}^{m\times k}$, $Q_j \equiv [q_1, \ldots, q_j] \in \mathbb{R}^{n\times j}$ (Q_0 represents a matrix with no columns); $L_{k,j} \equiv P_k^T A Q_j$ denotes the $k \times j$ leading principal block of L, in particular $L_{\overline{m},\overline{n}} = A_{11}$ (see (3.21)), and $l_{k,j} \equiv e_k^T L e_j$ is the (k,j)th entry of L. The variables c_U and c_L are counters of the upper and lower deflations, respectively. The algorithm stops when $c_U + c_L = \overline{d} = \mathrm{rank}(B)$; see the line 7. The indices j and k denote the number of columns and rows, respectively, of the currently computed part of the matrix L. If j or k becomes equal to n or m, respectively, then the algorithm stays in the loop of lines {7–13, 36–39, 7, etc.} or {7–26, 32–35, 38–39, 7, etc.}. The value of c_U respectively c_L increases until $c_U + c_L = \overline{d}$. The following schema illustrates (on the example given below (3.20)) how the algorithm assembles the matrix A_{11}; the arrows represent updates in the lines 24 or 31:

$$L_{\overline{d},0} = \left[\ \right] \xrightarrow{24} \begin{bmatrix} \alpha_{1,4} \\ \beta_{2,4} \\ \beta_{3,4} \end{bmatrix} \xrightarrow{31} \begin{bmatrix} \alpha_{1,4} \\ \beta_{2,4} \\ \beta_{3,4} \\ \hline \gamma_{4,4} \end{bmatrix} \xrightarrow{24} \left[\begin{array}{c|c} \alpha_{1,4} & 0 \\ \beta_{2,4} & \alpha_{2,5} \\ \beta_{3,4} & \beta_{3,5} \\ \cline{1-1} \gamma_{4,4} & \beta_{4,5} \end{array}\right] \xrightarrow{24} \left[\begin{array}{c|c|c} \alpha_{1,4} & 0 & 0 \\ \beta_{2,4} & \alpha_{2,5} & 0 \\ \beta_{3,4} & \beta_{3,5} & \alpha_{3,6} \\ \cline{1-1} \gamma_{4,4} & \beta_{4,5} & \beta_{4,6} \end{array}\right]$$

$$\xrightarrow{31} \left[\begin{array}{c|c|c} \alpha_{1,4} & 0 & 0 \\ \beta_{2,4} & \alpha_{2,5} & 0 \\ \beta_{3,4} & \beta_{3,5} & \alpha_{3,6} \\ \cline{1-1} \gamma_{4,4} & \beta_{4,5} & \beta_{4,6} \\ \hline \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \gamma_{5,6} \end{array}\right] \xrightarrow{24} \left[\begin{array}{c|c|c|c} \alpha_{1,4} & 0 & 0 & 0 \\ \beta_{2,4} & \alpha_{2,5} & 0 & 0 \\ \beta_{3,4} & \beta_{3,5} & \alpha_{3,6} & 0 \\ \cline{1-1} \gamma_{4,4} & \beta_{4,5} & \beta_{4,6} & \alpha_{4,7} \\ \cline{1-3} \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \gamma_{5,6} & \beta_{5,7} \end{array}\right]$$

$$\xrightarrow{31} \ldots \xrightarrow{24} \left[\begin{array}{c|c|c|c|c|c|c} \alpha_{1,4} & 0 & 0 & 0 & 0 & 0 & 0 \\ \beta_{2,4} & \alpha_{2,5} & 0 & 0 & 0 & 0 & 0 \\ \beta_{3,4} & \beta_{3,5} & \alpha_{3,6} & 0 & 0 & 0 & 0 \\ \cline{1-1} \gamma_{4,4} & \beta_{4,5} & \beta_{4,6} & \alpha_{4,7} & 0 & 0 & 0 \\ \cline{1-3} \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \gamma_{5,6} & \beta_{5,7} & \alpha_{5,8} & 0 & 0 \\ \cline{1-4} \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \gamma_{6,7} & \beta_{6,8} & 0 & 0 \\ \cline{1-5} \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \gamma_{7,8} & \alpha_{7,9} & 0 \\ \cline{1-6} \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \multicolumn{1}{c}{0} & \gamma_{8,9} & \alpha_{8,10} \end{array}\right] = L_{\overline{m},\overline{n}} = A_{11}.$$

The sums in (3.12), (3.14), or in (3.16), (3.18), are implemented in the lines 11 and 25, respectively. This implementation does not reflect, for simplicity, the structure of zero entries in the band matrix; i.e., as an example, the sum in the line 11 computes the full matrix-vector product of the matrix $[q_1, \ldots, q_{j-1}]$ with the last column of $L_{k,j-1}^T$.

Algorithm 1 (Band generalization of the Golub–Kahan bidiagonalization).

```
input $A \in \mathbb{R}^{m\times n}$,   $B \in \mathbb{R}^{m\times d}$      $\{A^T B \neq 0, \operatorname{rank}(B) = \overline{d}\}$
compute $B = [C, 0]R^T$      $\{$RHS preprocessing, $C \in \mathbb{R}^{m\times\overline{d}}$, $R^T = R^{-1}\}$
compute $C = P_{\overline{d}} F_1$      $\{$QR decomposition in the economic form$\}$
initialize $Q_0 \leftarrow [\,]$,   $L_{\overline{d},0} \leftarrow [\,]$      $\{$data arrays/matrices$\}$
initialize $c_U \leftarrow 0$,   $c_L \leftarrow 0$      $\{$deflation counters$\}$
initialize $j \leftarrow 1$,   $k \leftarrow \overline{d}$      $\{$control variables/indices$\}$
while   $c_U + c_L < \overline{d}$   do
   if   $j = 1$,   then      $\{$compute an auxiliary vector$\}$
      $\mathsf{aux}_q \leftarrow A^T p_{j+c_U} = A^T p_1$
   else
      $\mathsf{aux}_q \leftarrow A^T p_{j+c_U} - \sum_{i=1}^{j-1} q_i l_{j+c_U,i}$
   end
   if   $\mathsf{aux}_q \neq 0$,   then
      $\alpha_{j+c_U,\overline{d}+j} \leftarrow \|\mathsf{aux}_q\|$      $\{$compute $\alpha$ coefficient$\}$
      $q_j \leftarrow \mathsf{aux}_q / \alpha_{j+c_U,\overline{d}+j}$      $\{$compute $q$ vector$\}$
      $Q_j \leftarrow [Q_{j-1}, q_j]$      $\{$update of $Q$ matrix$\}$
      $\mathsf{beta} \leftarrow [\,]$
      if   $c_U + c_L < \overline{d} - 2$,   then
         for   $i = j + 1 + c_U, \ldots, j + \overline{d} - 1 - c_L$   do
            $\beta_{i,\overline{d}+j} \leftarrow p_i^T A q_j$      $\{$compute $\beta$ coefficients$\}$
            $\mathsf{beta} \leftarrow [\mathsf{beta}, \beta_{i,\overline{d}+j}]$
         end
      end
      $L_{k,j} \leftarrow [L_{k,j-1}, [0_{1,j-1+c_U}, \alpha_{j+c_U,\overline{d}+j}, \mathsf{beta}\,]^T]$      $\{$update of $L$ (add a col.)$\}$
      $\mathsf{aux}_p \leftarrow A q_j - \sum_{i=1}^{k} p_i l_{i,j}$      $\{$compute an auxiliary vector$\}$
      if   $\mathsf{aux}_p \neq 0$,   then
         $k \leftarrow k + 1$
         $\gamma_{k,\overline{d}+j} \leftarrow \|\mathsf{aux}_p\|$      $\{$compute $\gamma$ coefficient$\}$
         $p_k \leftarrow \mathsf{aux}_p / \gamma_{k,\overline{d}+j}$      $\{$compute $p$ vector$\}$
         $P_k \leftarrow [P_{k-1}, p_k]$      $\{$update of $P$ matrix$\}$
         $L_{k,j} \leftarrow [L_{k-1,j}^T, [0_{1,j-1}, \gamma_{k,\overline{d}+j}]^T]^T$      $\{$update of $L$ matrix (add a row)$\}$
      else
         $c_L \leftarrow c_L + 1$      $\{$lower deflation$\}$
      end
      $j \leftarrow j + 1$
   else
      $c_U \leftarrow c_U + 1$      $\{$upper deflation$\}$
   end
end
$\overline{m} \leftarrow k$, $\overline{n} \leftarrow j - 1$, $B_1 \leftarrow [F_1^T, 0_{\overline{d},\overline{m}-\overline{d}}]^T$, $A_{11} \leftarrow L_{\overline{m},\overline{n}}$, $P_1^{\mathrm{cp}} \leftarrow P_{\overline{m}}$, $Q_1^{\mathrm{cp}} \leftarrow Q_{\overline{n}}$
output $A_{11} \in \mathbb{R}^{\overline{m}\times\overline{n}}$,   $B_1 \in \mathbb{R}^{\overline{m}\times\overline{d}}$,   $P_1^{\mathrm{cp}} \in \mathbb{R}^{m\times\overline{m}}$,   $Q_1^{\mathrm{cp}} \in \mathbb{R}^{n\times\overline{n}}$,   $R \in \mathbb{R}^{d\times d}$
```