REPORT

A Divide-and-Conquer Method for Symmetric Banded Eigenproblems

Part I: Theoretical Results

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Abstract

The two currently most interesting methods for solving symmetric tridiagonal eigenproblems on parallel computers are (i) divide-and-conquer methods, and (ii) the so-called "Holy Grail" method (Dhillon [10]). None of these methods has been generalized for non-tridiagonal banded eigenproblems, i. e., problems with band matrices having more than one lower and upper side-diagonal, in a stable and efficient way.

The highly accurate eigenvalue calculation for tridiagonal matrices utilized in the "Holy Grail" method cannot be generalized directly to band matrices with more than three diagonals (Demmel and Gragg [9]). Thus, it is not clear at the moment whether the "Holy Grail" method can be adapted for non-tridiagonal banded eigenproblems. Generalizations of divide-and-conquer methods for banded eigenproblems have been investigated to some extent (Arbenz [2], Arbenz and Golub [4], Arbenz et al. [3]). However, until now no methods have been published which are efficient and numerically stable as well.

In this paper a divide-and-conquer scheme for symmetric banded eigenproblems is presented. It features a remarkably low computational complexity. In particular, computation of an orthogonal eigenbasis in the synthesis of two subproblems is a numerically stable non-iterative process of *quadratic* complexity.

Contents

Chapter 1

Introduction

The investigation and experimental evaluation of solvers for symmetric eigenproblems based on a two step reduction to tridiagonal form (Bischof et al. [5, 6], Gansterer et al. [15, 12, 13, 14]) led us to investigate efficient methods for banded eigenproblems (with usually small bandwidths), trying to avoid the second reduction step entirely.

In this paper the focus is on solving the standard symmetric eigenproblem for a band matrix with lower and upper bandwidth b, where usually $1 < b \ll n$. The "benchmark" the methods have to be evaluated against is conventional tridiagonalization of the band matrix followed by one of the well-known methods for solving the tridiagonal eigenproblem (see, for instance, Parlett [21] or Golub and Van Loan [17]) as implemented in standard software like LAPACK [1].

The Problem Setting

Given a symmetric band matrix $B \in \mathbb{R}^{n\times n}$ with semibandwidth b (b sub- and superdiagonals, respectively), compute the eigendecomposition (the symmetric real Schur decomposition)

$$B = V\Lambda V^{\top}.$$

B is orthogonally similar to the diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$.

Generalized Divide-and-Conquer Methods

The main emphasis of this paper will be on generalizations of the divide-and-conquer method (Cuppen [7], Dongarra and Sorensen [11], Gu and Eisenstat [18]) for band matrices with $b > 1$.

Two important related approaches have to be mentioned here: On the one hand, a generalized divide-and-conquer method to compute *approximate* eigenpairs of symmetric block tridiagonal matrices is currently being developed by Muller and Ward [20]. On the other hand, a few years ago important work has been done towards a divide-and-conquer method for band matrices (Arbenz and Golub [4], Arbenz et al. [3]). Unfortunately, methods developed based on this work exhibit unsatisfactory numerical accuracy, in particular with respect to the eigenvectors computed (Arbenz [2]).

In the following, a new divide-and-conquer method for band matrices will be developed. In contrast to the approach chosen by Muller and Ward [20], the goal of this paper is to derive methods for computing "exact" eigenpairs (except for rounding errors resulting from floating-point arithmetic). The new algorithm is based on theoretical considerations of Arbenz et al. [3]. Orthonormal eigenvectors of symmetric rank-b modifications of a diagonal matrix are calculated by a direct method of quadratic complexity.

The new algorithm has been developed in close analogy to the tridiagonal case as described in the literature (see, for instance, Demmel [8]) and similarities as well as differences will be emphasized in this paper wherever possible.

Chapter 2

The Divide-and-Conquer Process

Like the tridiagonal divide-and-conquer method, a banded divide-and-conquer method can be structured into (i) a subdivision step, (ii) a solution step, and (iii) a synthesis step.

2.1 The Subdivision Step

In analogy to the tridiagonal case, the band matrix B is divided into p smaller parts, each of them being a band matrix of size $n/p \times n/p$. For simplicity, only the case $p = 2$ is illustrated here.

It should be noted that there are several possibilities for subdividing the original problem, a summary of which is given in Arbenz [2]. For the moment, the description will be restricted to the following decomposition:

$$
\begin{aligned}
B &= \begin{pmatrix} B_1 & R^\top \\ R & B_2 \end{pmatrix} \\
&= \begin{pmatrix} B_1 - \begin{pmatrix} \mathbf{0} \\ I_b \end{pmatrix} & \mathbf{0} \\ \mathbf{0} & B_2 - \begin{pmatrix} RR^\top \\ \mathbf{0} \end{pmatrix} \end{pmatrix} + \\
&\quad + \begin{pmatrix} \mathbf{0} \\ I_b \\ R \\ \mathbf{0} \end{pmatrix} \left(\mathbf{0} \mid I_b \mid R^\top \mid \mathbf{0} \right) \\
&= \begin{pmatrix} \hat{B}_1 & \mathbf{0} \\ \mathbf{0} & \hat{B}_2 \end{pmatrix} + WW^\top.
\end{aligned}
$$

Here, $B_1, B_2, \hat{B}_1, \hat{B}_2$ are band matrices of size $n/2 \times n/2$, $R \in \mathbb{R}^{b \times b}$ is upper triangular and $W \in \mathbb{R}^{n \times b}$.

2.2 The Solution Step

The p smaller eigenproblems $\hat{B}_i x = \sigma x$ are solved independently, resulting in the factorizations

$$
\hat{B}_i = Q_i \Sigma_i Q_i^\top, \quad i = 1, 2, \ldots, p. \tag{2.1}
$$

This can be done using any suitable method (see Parlett [21] or Golub and Van Loan [17]); for instance, by tridiagonalizing $\hat{B}_i$ and then solving the resulting tridiagonal eigenproblem.

2.3 The Synthesis Step

The matrix of eigenvectors V and the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of B are computed utilizing the factorizations obtained in the solution step. This computation can be organized in a tree-structure, where in each step "neighboring" pairs are combined using the factorizations (2.1). For $p = 2$

$$\begin{aligned} B &= \begin{pmatrix} Q_1 \Sigma_1 Q_1^\top & \mathbf{0} \\ \mathbf{0} & Q_2 \Sigma_2 Q_2^\top \end{pmatrix} + WW^\top \\ &= \begin{pmatrix} Q_1 & \mathbf{0} \\ \mathbf{0} & Q_2 \end{pmatrix} \left[\begin{pmatrix} \Sigma_1 & \\ & \Sigma_2 \end{pmatrix} + UU^\top \right] \begin{pmatrix} Q_1^\top & \mathbf{0} \\ \mathbf{0} & Q_2^\top \end{pmatrix}. \end{aligned} \tag{2.2}$$

Using the partitionings

$$W = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix}, W_1 = \begin{pmatrix} \mathbf{0} \\ I_b \end{pmatrix}, W_2 = \begin{pmatrix} R \\ \mathbf{0} \end{pmatrix}, \quad \text{and} \quad U = \begin{pmatrix} U_1 \\ U_2 \end{pmatrix}$$

the relationships $W_1 = Q_1 U_1$ and $W_2 = Q_2 U_2$ hold. Thus, U_1 consists of the b last rows of Q_1, and U_2 consists of linear combinations of the b first rows of Q_2. Hence, only the b last rows of Q_1 and the b first rows of Q_2 have to be known.

The main problem of the synthesis-step of a divide-and-conquer algorithm for band matrices is to synthesize the eigensystem of the band matrix B from the computed eigensystems of the two parts $\hat{B}_1$ and $\hat{B}_2$.

In the tridiagonal case, this step comprises the computation of the eigenvalues and eigenvectors of a matrix $\Sigma + \alpha u u^\top$, where $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$, and $u \in \mathbb{R}^n$. This problem can be reduced to computing the determinant of a rank-one modification of the identity matrix, i. e., of a matrix $I_n + xy^\top$, which can be done very efficiently (Demmel [8]).

The central complication in the general banded case is that the method used for the eigenanalysis of a rank-one modification of a diagonal matrix cannot be generalized directly to a rank-b modification with $b > 1$.

Arbenz and Golub [4] and Arbenz et al. [3] provide many important theoretical results concerning the eigenanalysis of a rank-b modification of a diagonal matrix. In particular, they suggest an approach which reduces the eigenanalysis of a rank-b modification of a diagonal matrix to a (small) $b \times b$ eigenproblem using a cleverly chosen *equivalence* transformation (cf. (4.18) and (4.19)). Unfortunately, at present it is not clear how this methodology could be used successfully in algorithms for banded eigenproblems. Numerical instabilities in the computation of the eigenvectors have been observed (Arbenz [2]), and currently no numerically stable implementation exists.

Eigenanalysis of the Synthesis Matrix

The most important subproblem of divide-and-conquer algorithms is to compute the eigenvalues and eigenvectors of the *synthesis matrix*

$$S := \Sigma + UU^\top \quad \in \mathbb{R}^{n\times n}, \tag{2.3}$$

where $\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_n)$ with ordered entries $\sigma_1 \le \sigma_2 \le \ldots \le \sigma_n$, $U = (u_1 \mid u_2 \mid \cdots \mid u_b) \in \mathbb{R}^{n\times b}$, and $\mathrm{rank}(U) = b$.

Different methods for computing the eigenvalues and eigenvectors of low rank modifications of a Hermitian matrix are summarized in Arbenz [2]. Two basic approaches can be distinguished.

The $\mathbf{1 \times b}$ Approach. The idea of this approach is to compress the rank-b modification to a $b \times b$ problem and to reconstruct the solution of the original problem from the solution of the smaller problem. The underlying theoretical concept is described in Arbenz and Golub [4] and Arbenz et al. [3].

The $\mathbf{b \times 1}$ Approach. The idea of this alternative approach is to perform the rank-b modification as a sequence of b rank-one modifications (Arbenz [2]).

The $b \times 1$ approach (which was considered by Arbenz [2]) requires significantly more floating-point operations than the $1 \times b$ approach and is therefore not competitive. Moreover, the $1 \times b$ approach produces results with unsatisfactory accuracy. In Arbenz' experiments, the eigenvectors computed did not satisfy the required orthogonality conditions. To overcome this shortcoming Arbenz suggested modifications to stabilize his algorithm. However, the stabilized versions turned out to be less efficient than the standard algorithm, i. e., tridiagonalization followed by solution of the tridiagonal eigenproblem (Arbenz [2]).

The new approach for performing the synthesis step in a generalized divide-and-conquer method is based on the $b \times 1$ approach. In Chapter 3 it will be shown how to avoid the algorithmic overhead which led to the rejection of this approach by Arbenz [2] and to construct an $O(n^2)$ method (for $b \ll n$), which allows to compute numerically orthogonal eigenvectors (see Chapter 4).

Chapter 3

Computation of the Eigenvalues

In this chapter methods are discussed how to compute the eigenvalues $\sigma_1^*, \sigma_2^*, \ldots, \sigma_n^*$ of the synthesis matrix S as defined in (2.3).

Based on the fact that

$$\Sigma + UU^\top = \Sigma + \sum_{i=1}^{b} u_i u_i^\top$$

the eigenvalues of S can be computed in b successive steps. Each of these steps involves the eigenanalysis of a rank-one modification of a diagonal matrix and is closely related to the synthesis step of the tridiagonal divide-and-conquer method (Cuppen [7], Gu and Eisenstat [18]).

Step 1. For the newly defined matrix $A_1 := \Sigma + u_1 u_1^\top$ an eigenanalysis is performed which results in the factorization $A_1 = Q_1 \Sigma_1 Q_1^\top, \quad Q_1^\top Q_1 = I_n$.

Step 2. For $A_2 := \Sigma_1 + Q_1^\top u_2 u_2^\top Q_1$ an eigenanalysis is performed which results in the factorization $A_2 = Q_2 \Sigma_2 Q_2^\top, \quad Q_2^\top Q_2 = I_n$.

$\vdots$

Step b. For $A_b := \Sigma_{b-1} + Q_{b-1}^\top \cdots Q_1^\top u_b u_b^\top Q_1 \cdots Q_{b-1}$ an eigenanalysis is performed which results in the factorization $A_b = Q_b \Sigma_b Q_b^\top, \quad Q_b^\top Q_b = I_n$.

After carrying out these steps the eigendecomposition

$$\Sigma + UU^\top = (Q_1 Q_2 \cdots Q_b) \Sigma_b (Q_1 Q_2 \cdots Q_b)^\top \tag{3.1}$$

has been computed (which can be seen by successive back substitution). This implies two remarkable features of the algorithm comprising the b steps described above.

- The entries of the diagonal matrix Σ_b are the same as those of the eigenvalue matrix

  $$\Sigma^* = \mathrm{diag}(\sigma_1^*, \sigma_2^*, \ldots, \sigma_n^*)$$

  of S. For $b \ll n$, the eigenvalues of S can therefore be computed with $O(n^2)$ operations.

- An orthogonal set of eigenvectors of S is available *explicitly* from (3.1) in the form of the product $Q_1 Q_2 \cdots Q_b$. Its computation from this representation, however, is an $O(n^3)$ operation, which has to be avoided.

Consequently, this algorithm will be used only for computing the eigenvalues of the synthesis matrix S, and alternatively, more efficient methods will be applied for computing the eigenvectors of S (see Chapter 4).

Parallelization

The preceding algorithm can be "quasi"-parallelized. Once Q_1 is known, the $b-1$ matrix-vector products

$$Q_1^\top u_2,\ Q_1^\top u_3, \cdots, Q_1^\top u_b$$

can be computed in parallel. Once Q_2 is known, the $b-2$ products

$$Q_2^\top \left(Q_1^\top u_3\right),\ Q_2^\top \left(Q_1^\top u_4\right), \cdots, Q_2^\top \left(Q_1^\top u_b\right)$$

can be computed in parallel, et cetera.

Chapter 4

Computation of the Eigenvectors

In this chapter methods are discussed how to compute the eigenvectors $v_1^*, v_2^*, \ldots, v_n^*$ of the synthesis matrix S as defined in (2.3), given the eigenvalues $\sigma_1^*, \sigma_2^*, \ldots, \sigma_n^*$ of S as computed in Section 3.

The main goal is to compute a full set of orthonormal eigenvectors using only $O(n^2)$ operations (for $b \ll n$). In order to achieve this goal, explicit reorthogonalization may only be used on very small sets of eigenvectors. Two different approaches are possible.

1. Computing the eigenvectors directly using newly developed explicit formulas;
2. Performing inverse iteration applied to the matrix $\Sigma + UU^\top$ (see Gansterer et al. [16]).

The latter approach in its standard form may fail to achieve the goal of applying only $O(n^2)$ operations in case reorthogonalization is required (Dhillon [10]), and therefore the former approach will be pursued in this report.

In this chapter it will be shown how an orthonormal basis for the eigenspace of S can be constructed. Since eigenvectors corresponding to distinct eigenvalues are orthogonal (Horn and Johnson [19]) only an orthonormal basis of the eigenspace corresponding to one given eigenvalue σ_i^* has to be constructed.

Three cases have to be distinguished.

Case I

In the first case assume that $\sigma_i^* \notin \lambda(\Sigma)$ and has an algebraic multiplicity l, $1 \leq l \leq b$. Since σ_i^* is an eigenvalue of S, the matrix $\Sigma + UU^\top - \sigma_i^* I_n$ is singular. This implies the existence of an n-vector $x \neq 0$ (a corresponding eigenvector), such that

$$\left(\Sigma + UU^\top - \sigma_i^* I_n\right) x = \mathbf{0}.$$

Premultiplication with $(\Sigma - \sigma_i^* I_n)^{-1}$ (which exists because of the assumption $\sigma_i^* \notin \lambda(\Sigma)$) yields

$$\left(I_n + (\Sigma - \sigma_i^* I_n)^{-1} UU^\top\right) x = \mathbf{0}.$$

It follows that

$$I_n + (\Sigma - \sigma_i^* I_n)^{-1} UU^\top$$

is a singular matrix. Similarly, premultiplication with $U^\top (\Sigma - \sigma_i^* I_n)^{-1}$ yields

$$\left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^{-1} U\right) U^\top x = \mathbf{0}, \tag{4.1}$$

which shows that

$$I_b + U^\top (\Sigma - \sigma_i^* I_n)^{-1} U \tag{4.2}$$

is a singular matrix. The singularity of (4.2) implies

$$Q_i^\top \left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^{-1} U\right) P_i = \begin{pmatrix} R_{i1} & R_{i2} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \tag{4.3}$$

i. e., a QR factorization with column pivoting (Golub and Van Loan [17]) with $1 \leq m \leq b$, an orthonormal matrix $Q_i \in \mathbb{R}^{b\times b}$, a permutation matrix $P_i \in \mathbb{R}^{b\times b}$ (i. e., $Q_i^\top Q_i = P_i^\top P_i = I_b$), a nonsingular upper triangular matrix $R_{i1} \in \mathbb{R}^{(b-m)\times(b-m)}$, and a matrix $R_{i2} \in \mathbb{R}^{(b-m)\times m}$. The matrix

$$X_i := P_i \begin{pmatrix} -R_{i1}^{-1} R_{i2} \\ I_m \end{pmatrix} \quad \in \mathbb{R}^{b\times m} \tag{4.4}$$

has rank m and (because of (4.3)) its columns span the null space of (4.2), i. e.,

$$\left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^{-1} U\right) X_i = \mathbf{0}. \tag{4.5}$$

Computation of the Eigenvectors. Compute the QR factorization of the $n \times m$ matrix

$$(\Sigma - \sigma_i^* I_n)^{-1} U X_i = Z_i S_i \tag{4.6}$$

with $Z_i \in \mathbb{R}^{n\times m}$ and nonsingular upper triangular $S_i \in \mathbb{R}^{m\times m}$. The column vectors of Z_i form a set of l orthonormal eigenvectors of S. From

$$\begin{aligned} \left(\Sigma + UU^\top - \sigma_i^* I_n\right) Z_i &= \\ UU^\top (\Sigma - \sigma_i^* I_n)^{-1} U X_i S_i^{-1} + U X_i S_i^{-1} &= \\ U\left(U^\top (\Sigma - \sigma_i^* I_n)^{-1} U + I_b\right) X_i S_i^{-1} &= \mathbf{0} \quad \text{according to (4.5)} \end{aligned}$$

it follows that $\left(\Sigma + UU^\top\right) Z_i = \sigma_i^* Z_i$, i. e., the columns of Z_i are eigenvectors of S corresponding to σ_i^*. They are orthonormal by construction.

It remains to be shown that *all* l eigenvectors corresponding to the eigenvalue σ_i^* have been found, that is, $m = l$. First, since the geometric multiplicity of an eigenvalue is less or equal its algebraic multiplicity (Horn and Johnson [19]), $m \leq l$. Equality can be shown indirectly. Assume that $m < l$. Then there must be another eigenvector z_i of S with $\|z_i\|_2 = 1$, $z_i^\top Z_i = \mathbf{0}$, and, according to (4.1),

$$\begin{aligned} \left(\Sigma + UU^\top - \sigma_i^* I_n\right) z_i &= \mathbf{0} \\ \left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^{-1} U\right) U^\top z_i &= \mathbf{0}. \end{aligned} \tag{4.7}$$

This implies that $U^\top z_i$ lies in the null space of

$$I_b + U^\top (\Sigma - \sigma_i^* I_n)^{-1} U,$$

and since X_i is a basis of this null space (according to (4.5)), there exists a vector $y \in \mathbb{R}^m$ such that $U^\top z_i = X_i y$. Thus

$$(\Sigma - \sigma_i^* I_n)^{-1} UU^\top z_i = (\Sigma - \sigma_i^* I_n)^{-1} U X_i y = (4.6) = Z_i S_i y.$$

Consequently,

$$z_i^\top \left(\Sigma - \sigma_i^* I_n\right)^{-1} U U^\top z_i = z_i^\top Z_i S_i y = 0,$$

but according to (4.7) also

$$z_i^\top \left(\Sigma - \sigma_i^* I_n\right)^{-1} U U^\top z_i = z_i^\top \left(\Sigma - \sigma_i^* I_n\right)^{-1} \left(-\left(\Sigma - \sigma_i^* I_n\right)\right) z_i = -\|z_i\|_2^2,$$

which leads to the contradiction $\|z_i\|_2 = 0$.

Case II

In the second case assume that $\sigma_i^* \notin \lambda(\Sigma)$ and has an algebraic multiplicity l, $b+1 \leq l \leq n$. It turns out that this case cannot occur, which can be proved indirectly.

Assume that $l \geq b+1$. Then σ_i^* is also a b-fold eigenvalue and because $m = l$ the QR factorization with column pivoting (4.3) "degenerates" to

$$Q_i^\top \left(I_b + U^\top \left(\Sigma - \sigma_i^* I_n\right)^{-1} U\right) P_i = \mathbf{0}, \tag{4.8}$$

which implies that

$$\left(I_b + U^\top \left(\Sigma - \sigma_i^* I_n\right)^{-1} U\right) = \mathbf{0} \tag{4.9}$$

and that $X_i = P_i I_m = P_i$. Therefore, Z_i defined by (4.6) has b columns which form an orthonormal eigensystem.

Let $\hat{U} \in \mathbb{R}^{n \times (n-b)}$ denote the orthogonal complement of U with orthonormal columns, i. e.,

$$\hat{U}^\top U = \mathbf{0} \qquad \text{and} \qquad \hat{U}^\top \hat{U} = I_{n-b}. \tag{4.10}$$

If the multiplicity of σ_i^* were larger than b, there would be at least one (nonzero) eigenvector of S orthogonal to Z_i. Representing this eigenvector in terms of the orthogonal subspaces U and $\hat{U}$ as $(x^\top \mid y^\top)^\top$ with $x \in \mathbb{R}^b$, $y \in \mathbb{R}^{n-b}$, and denoting $V := (\Sigma - \sigma_i^* I_n)^{-1} U$, implies

$$\left(I_n + V U^\top\right) \left(U x + \hat{U} y\right) = \mathbf{0} \tag{4.11}$$

and

$$\left(U x + \hat{U} y\right)^\top Z_i = \mathbf{0}.$$

Since $Z_i = V P_i S_i^{-1}$ with regular P_i and S_i it follows that

$$\begin{aligned} \left(U x + \hat{U} y\right)^\top V &= \mathbf{0} \\ x^\top U^\top V + y^\top \hat{U}^\top V &= \mathbf{0}. \end{aligned}$$

Since (4.9) implies that $I_b + U^\top V = \mathbf{0}$ this leads to

$$x = V^\top \hat{U} y. \tag{4.12}$$

Substituting (4.12) into (4.11) yields

$$\left(UV^\top + V\left(U^\top U\right)V^\top + I_n\right)\hat{U}y = \mathbf{0}. \tag{4.13}$$

Multiplication by $V^\top$ from the left and (again) utilizing $V^\top U + I_b = \mathbf{0}$, which follows from (4.9), leads to

$$\left(V^\top V\right)\left(U^\top U\right)V^\top \hat{U}y = \mathbf{0}. \tag{4.14}$$

$V^\top V$ and $U^\top U$ are regular matrices and therefore

$$V^\top \hat{U}y = (4.12) = x = \mathbf{0}. \tag{4.15}$$

Substituting (4.15) into (4.11) implies $\hat{U}y = \mathbf{0}$, and therefore $y = \mathbf{0}$, which contradicts the assumption of a nonzero eigenvector. Therefore, if $\sigma_i^* \notin \lambda(\Sigma)$ then its algebraic multiplicity is at most equal to b. Thus, the second case can be excluded from further considerations.

Case III

In the third case assume that $\sigma_i^* \in \lambda(\Sigma) \cap \lambda(S)$. Further assume that σ_i^* has an algebraic multiplicity r in $\lambda(\Sigma)$ and l in $\lambda(S)$. If

$$W_i := \begin{pmatrix} \mathbf{0} \\ I_r \\ \mathbf{0} \end{pmatrix} \quad \in \mathbb{R}^{n\times r} \tag{4.16}$$

then its orthonormal columns form a basis of the null space of $\Sigma - \sigma_i^* I_n$, i. e.,

$$\left(\Sigma - \sigma_i^* I_n\right) W_i = \mathbf{0}, \tag{4.17}$$

so

$$\left(\Sigma - \sigma_i^* I_n\right)\left(\Sigma - \sigma_i^* I_n\right)^+ = I_n - W_i W_i^\top.$$

The two quadratic matrices

$$A_i := \begin{pmatrix} -\left(\Sigma - \sigma_i^* I_n + UU^\top\right) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & I_b & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{4.18}$$

and

$$B_i := \begin{pmatrix} -\left(\Sigma - \sigma_i^* I_n\right) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & I_b + U^\top\left(\Sigma - \sigma_i^* I_n\right)^+ U & U^\top W_i \\ \mathbf{0} & W_i^\top U & \mathbf{0} \end{pmatrix} \tag{4.19}$$

are congruent (Arbenz et al. [3]), and therefore they have the same inertia (Horn and Johnson [19]). In particular, the number ξ of their zero eigenvalues is the same. The definition

$$R_i := \begin{pmatrix} I_b + U^\top\left(\Sigma - \sigma_i^* I_n\right)^+ U & U^\top W_i \\ W_i^\top U & \mathbf{0} \end{pmatrix}$$

implies

$$\xi(A_i) = l + r = \xi(B_i) = r + \xi(R_i). \tag{4.20}$$

This implies that $\xi(R_i) = l$, and, since $l \geq 1$, that R_i is singular, and that $l \leq b+r$. Consequently, there exists a matrix $\left(X_i^\top \mid Y_i^\top\right)^\top$ of rank l with $X_i \in \mathbb{R}^{b\times l}$ and $Y_i \in \mathbb{R}^{r\times l}$, such that

$$R_i \begin{pmatrix} X_i \\ Y_i \end{pmatrix} = \mathbf{0}, \tag{4.21}$$

or, equivalently,

$$\begin{aligned} \left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^+ U\right) X_i + U^\top W_i Y_i &= \mathbf{0} && (4.22)\\ W_i^\top U X_i &= \mathbf{0}. && (4.23) \end{aligned}$$

Computation of the Eigenvectors. Given the null space $\left(X_i^\top \mid Y_i^\top\right)^\top$ of R_i (a discussion of how it can be computed will be deferred for the moment), define

$$\hat{Z}_i := (\Sigma - \sigma_i^* I_n)^+ U X_i + W_i Y_i \quad \in \mathbb{R}^{n\times l}. \tag{4.24}$$

The columns of $\hat{Z}_i$ form a set of l linearly independent eigenvectors of S corresponding to σ_i^*. Because of (4.23) and (4.17)

$$\begin{aligned} \left(\Sigma + UU^\top - \sigma_i^* I_n\right) \hat{Z}_i &= \\ U X_i + UU^\top (\Sigma - \sigma_i^* I_n)^+ U X_i + UU^\top W_i Y_i &= \\ U\left(\left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^+ U\right) X_i + U^\top W_i Y_i\right) &= \mathbf{0} \quad \text{according to (4.22).} \end{aligned}$$

Because of

$$\operatorname{rank}(\hat{Z}_i) = l, \tag{4.25}$$

the columns of $\hat{Z}_i$ span the whole eigenspace corresponding to σ_i^*. (4.25) can be proved indirectly. Assume, that $\operatorname{rank}(\hat{Z}_i) < l$. Then there must be another eigenvector $z_i \in \mathbb{R}^n$ with

$$\|z_i\|_2 = 1, \qquad z_i^\top \hat{Z}_i = \mathbf{0},$$

and

$$\left(\Sigma + UU^\top - \sigma_i^* I_n\right) z_i = \mathbf{0}. \tag{4.26}$$

Premultiplication with $U^\top (\Sigma - \sigma_i^* I_n)^+$ implies

$$\left(I_b + U^\top (\Sigma - \sigma_i^* I_n)^+ U\right) U^\top z_i - U^\top W_i W_i^\top z_i = \mathbf{0}. \tag{4.27}$$

At the same time, (4.26) implies

$$UU^\top z_i = -(\Sigma - \sigma_i^* I_n) z_i, \tag{4.28}$$

and premultiplication by $W_i^\top$ (using(4.17)) yields

$$W_i^\top UU^\top z_i = -W_i^\top (\Sigma - \sigma_i^* I_n) z_i = \mathbf{0}. \tag{4.29}$$

Comparing (4.27) and (4.29) with (4.22) and (4.23) reveals that the vector

$$\begin{pmatrix} U^\top \\ -W_i^\top \end{pmatrix} z_i$$

lies in the null space of R_i. Since this null space is spanned by $\left(X_i^\top \mid Y_i^\top\right)^\top$ (see (4.21)), there must be a vector $v \in \mathbb{R}^l$, such that

$$\begin{pmatrix} U^\top \\ -W_i^\top \end{pmatrix} z_i = \begin{pmatrix} X_i \\ Y_i \end{pmatrix} v.$$

Multiplying from the left with $z_i^\top \left((\Sigma - \sigma_i^* I_n)^+ U \mid W_i\right) \in \mathbb{R}^{1\times(b+r)}$ yields on the one hand

$$\begin{aligned} z_i^\top \left((\Sigma - \sigma_i^* I_n)^+ U \mid W_i\right) \begin{pmatrix} U^\top \\ -W_i^\top \end{pmatrix} z_i &= \\ z_i^\top \left((\Sigma - \sigma_i^* I_n)^+ U \mid W_i\right) \begin{pmatrix} X_i \\ Y_i \end{pmatrix} v &= (4.24) = \\ z_i^\top \hat{Z}_i v &= 0, \end{aligned}$$

and on the other hand

$$\begin{aligned} z_i^\top \left((\Sigma - \sigma_i^* I_n)^+ U \mid W_i\right) \begin{pmatrix} U^\top \\ -W_i^\top \end{pmatrix} z_i &= \\ z_i^\top \left((\Sigma - \sigma_i^* I_n)^+ U U^\top - W_i W_i^\top\right) z_i &= (4.28) = \\ z_i^\top \left(-I_n + W_i W_i^\top - W_i W_i^\top\right) z_i &= -\|z_i\|_2^2. \end{aligned}$$

This leads to $\|z_i\|_2 = 0$, in contradiction to the assumptions.

The columns of $\hat{Z}_i$ are not necessarily orthogonal. For large values of l explicit reorthogonalization might require an $O(n^3)$ effort. Therefore, special ways of representing the null space of R_i and thus computing an orthonormal set of l eigenvectors will be illustrated. These methods reorthogonalize only small blocks of eigenvectors, therefore retaining the overall quadratic complexity.

$\mathbf{r \le b}$. Since $l \le r + b$, $l \le 2b$ follows. By establishing a QR factorization with column pivoting of R_i,

$$Q_i^\top R_i P_i = \begin{pmatrix} S_{i1} & S_{i2} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

with S_{i1} being a regular upper triangular matrix, and partitioning

$$P_i \begin{pmatrix} -S_{i1}^{-1} S_{i2} \\ I_l \end{pmatrix} =: \begin{pmatrix} X_i \\ Y_i \end{pmatrix}$$

with $X_i \in \mathbb{R}^{b\times l}$, $Y_i \in \mathbb{R}^{r\times l}$ a basis of the null space of R_i has been found, i. e.,

$$R_i \begin{pmatrix} X_i \\ Y_i \end{pmatrix} = \mathbf{0}$$

and

$$\operatorname{rank}\left(\left(\begin{array}{c} X_i \\ Y_i \end{array}\right)\right) = l.$$

With a QR factorization of $\hat{Z}_i$ (defined by (4.24))

$$\hat{Z}_i = Z_i M_i,\ \ Z_i \in \mathbb{R}^{n\times l},\ \ M_i \in \mathbb{R}^{l\times l},$$

it holds that

$$Z_i^\top Z_i = I_l \quad \text{and} \quad \left(\Sigma - \sigma_i^* I_n + UU^\top\right) Z_i = \mathbf{0}.$$

$\mathbf{b+1 \le r \le n}$. The QR factorization

$$W_i^\top U = (Q_{i1} \mid Q_{i2}) \left(\begin{array}{c} L_i \\ \mathbf{0} \end{array}\right), \tag{4.30}$$

and the QR factorization with column pivoting

$$H_i^\top \left(\begin{array}{cc} E_i & L_i^\top \\ L_i & \mathbf{0} \end{array}\right) P_i = \left(\begin{array}{cc} T_{i1} & T_{i2} \\ \mathbf{0} & \mathbf{0} \end{array}\right), \quad p + q = 2b, \tag{4.31}$$

using the abbreviation $E_i := I_b + U^\top \left(\Sigma - \sigma_i^* I_n\right)^+ U$, imply that the upper triangular matrix T_{i1} is regular and with

$$\left(\begin{array}{c} \hat{X}_i \\ \hat{Y}_i \end{array}\right) := P_i \left(\begin{array}{c} -T_{i1}^{-1} T_{i2} \\ I_q \end{array}\right), \quad \hat{X}_i, \hat{Y}_i \in \mathbb{R}^{b\times q},$$

it follows that

$$\left(\begin{array}{cc} E_i & L_i^\top \\ L_i & \mathbf{0} \end{array}\right) \left(\begin{array}{c} \hat{X}_i \\ \hat{Y}_i \end{array}\right) = \mathbf{0} \quad \text{and} \quad \operatorname{rank}\left(\left(\begin{array}{c} \hat{X}_i \\ \hat{Y}_i \end{array}\right)\right) = q.$$

$\left(\Sigma - \sigma_i^* I_n + UU^\top\right) W_i Q_{i2} = \mathbf{0}$ because of (4.16) and $U^\top W_i Q_{i2} = \mathbf{0}$ because of (4.30). From (4.30) and (4.31) it follows that $K_1 K_2 = \mathbf{0}$ with

$$\begin{aligned} K_1 &:= \left(\begin{array}{cc} H_i^\top & \mathbf{0} \\ \mathbf{0} & I_{r-b} \end{array}\right) \left(\begin{array}{cc} I_b & \mathbf{0} \\ \mathbf{0} & Q_{i1}^\top \\ \mathbf{0} & Q_{i2}^\top \end{array}\right) \left(\begin{array}{cc} E_i & U^\top W_i \\ W_i^\top U & \mathbf{0} \end{array}\right) \\ K_2 &:= \left(\begin{array}{ccc} I_b & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & Q_{i1} & Q_{i2} \end{array}\right) \left(\begin{array}{cc} P_i & \mathbf{0} \\ \mathbf{0} & I_{r-b} \end{array}\right) \left(\begin{array}{cc} -T_{i1}^{-1} T_{i2} & \mathbf{0} \\ I_q & \mathbf{0} \\ \mathbf{0} & I_{r-b} \end{array}\right) \end{aligned}$$

and that

$$R_i \left(\begin{array}{cc} \hat{X}_i & \mathbf{0} \\ Q_{i1}\hat{Y}_i & Q_{i2} \end{array}\right) = \mathbf{0},$$

so $l = q + r - b$ and

$$\operatorname{rank}\left(\left(\begin{array}{cc} \hat{X}_i & \mathbf{0} \\ Q_{i1}\hat{Y}_i & Q_{i2} \end{array}\right)\right) = l.$$

With another QR factorization,

$$(\Sigma - \sigma_i^* I_n)^+ U\hat{X}_i + W_i Q_{i1}\hat{Y}_i = N_i F_i,$$

where $N_i \in \mathbb{R}^{n\times q}$, $N_i^\top N_i = I_q$, $F_i \in \mathbb{R}^{q\times q}$ is an upper triangular matrix, with $X_i := \left(\hat{X}_i \mid \mathbf{0}\right) \in \mathbb{R}^{b\times l}$, $Y_i := \left(Q_{i1}\hat{Y}_i \mid Q_{i2}\right) \in \mathbb{R}^{r\times l}$, the matrix $\hat{Z}_i$ (defined by (4.24)) satisfies

$$\left(\Sigma - \sigma_i^* I_n + UU^\top\right)\hat{Z}_i \quad = \quad \mathbf{0} \quad \text{and} \quad \operatorname{rank}(\hat{Z}_i) = l,$$

and can be represented as

$$\begin{aligned} \hat{Z}_i &= \left((\Sigma - \sigma_i^* I_n)^+ U \mid W_i\right)\begin{pmatrix} X_i \\ Y_i \end{pmatrix} \\ &= \left((\Sigma - \sigma_i^* I_n)^+ U\hat{X}_i + W_i Q_{i1}\hat{Y}_i \mid W_i Q_{i2}\right) \\ &= \left(N_i F_i \mid W_i Q_{i2}\right). \end{aligned}$$

Since $\operatorname{rank}(\hat{Z}_i) = l$, F_i must be nonsingular so with $Z_i := (N_i \mid W_i Q_{i2}) \in \mathbb{R}^{n\times l}$,

$$\left(\Sigma - \sigma_i^* I_n + UU^\top\right) Z_i = \left(\Sigma - \sigma_i^* I_n + UU^\top\right)\hat{Z}_i \begin{pmatrix} F_i^{-1} & \mathbf{0} \\ \mathbf{0} & I_{r-q} \end{pmatrix} = \mathbf{0}$$

and

$$Z_i^\top Z_i = I_l,$$

since

$$\begin{aligned} Q_{i2}^\top W_i N_i &= Q_{i2}^\top W_i \left((\Sigma - \sigma_i^* I_n)^+ U\hat{X}_i + W_i Q_{i1}\hat{Y}_i\right) F_i^{-1} \\ &= \left(Q_{i2}^\top W_i (\Sigma - \sigma_i^* I_n)^+ U\hat{X}_i + Q_{i2}^\top Q_{i1}\hat{Y}_i\right) F_i^{-1} \\ &= \mathbf{0}, \end{aligned}$$

because of (4.16).

Chapter 5

Summary

The development and implementation of efficient methods for solving banded eigenproblems on high-performance architectures is one of the challenging problems in numerical linear algebra.

This report points out new ways towards highly efficient and numerically stable eigensolvers for band matrices. The goal is to overcome difficulties which have been faced in previous attempts.

Algorithmic aspects of the new method are discussed in an accompanying report (Gansterer et al. [16]). Numerical aspects and implementation details are discussed in a forthcoming report.

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