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Recursive approximation of the dominant eigenspace of an indefinite matrix☆

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ABSTRACT

We consider here the problem of tracking the dominant eigenspace of an indefinite matrix by updating recursively a rank k approximation of the given matrix. The tracking uses a window of the given matrix, which increases at every step of the algorithm. Therefore, the rank of the approximation increases also, and hence a rank reduction of the approximation is needed to retrieve an approximation of rank k. In order to perform the window adaptation and the rank reduction in an efficient manner, we make use of a new anti-triangular decomposition for indefinite matrices. All steps of the algorithm only make use of orthogonal transformations, which guarantees the stability of the intermediate steps. We also show some numerical experiments to illustrate the performance of the tracking algorithm.

1. Introduction and notations

Indefinite symmetric matrices occur in many applications, such as optimization, partial differential equations and variational problems where they are for instance linked to a so-called saddle point problem. In these applications one is often interested in tracking the subspace associated to the largest eigenvalues. We consider in this paper the problem of tracking the dominant eigenspace of an indefinite matrix by updating recursively a low rank approximation of the given matrix. The proposed algorithm can be used, for instance, for problems where at each time instant a new row and column is appended to the existing symmetric indefinite matrix, and the knowledge of the dominant subspace is required.

In the sequel, we introduce the basic notations used in this paper. The *inertia* of a symmetric matrix $A \in \mathbb{R}^{n\times n}$ is the triple $\text{Inertia}(A) = (n_-, n_0, n_+)$, where n_-, n_0 and n_+ are the number of negative, zero and positive eigenvalues of A, respectively, and $n_- + n_0 + n_+ = n$. The identity matrix of order n is denoted by I_n and its columns, the unit vectors, are denoted by $\mathbf{e}_i^{(n)}$, $i = 1, \ldots, n$. Submatrices are denoted by the colon notation of MATLAB: $A(i : j, k : l)$ denotes the submatrix of A formed by the intersection of rows i to j and columns k to l, and $A(i : j, :)$ denotes the rows of A from i to j. Vectors are usually denoted in bold. A null submatrix is denoted by $\mathbf{0}$ and its size can vary depending on the context.

The paper is organized as follows. In Section 2, we consider the problem of finding the dominant eigenspace of a bordered symmetric matrix. This amounts to computing the k-dimensional subspace associated to the largest eigenvalues in absolute value of a bordered symmetric matrix, when we have an approximation of the dominant subspace of the smaller matrix. Based on this "updating" algorithm, an iterative procedure for tracking the dominant eigenspace of an indefinite matrix is

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proposed. In Section 3 we derive some bounds for the accuracy that can be obtained with our method. In Section 4 we present some numerical experiments illustrating that the algorithm is numerically stable and that the eigenvalues and eigenvectors are well approximated as the recursion proceeds.

2. Bordering problem

Let $A_i := A(1:i, 1:i)$, $i = 1, \ldots, n$. Suppose we have a rank–k approximation of A_i, $1 \le k \le i \le n$ of the form

$$A_i \approx U_i M_i U_i^T =: \tilde{A}_i,$$

with $M_i \in \mathbb{R}^{k\times k}$ symmetric and $U_i \in \mathbb{R}^{i\times k}$ with orthonormal columns.

The main idea is to obtain a rank–k approximation of A_{i+1} by using the best rank–k approximation in Frobenius norm as well as in spectral norm of another bordered matrix, namely

$$\hat{A}_{i+1} = \begin{bmatrix} \tilde{A}_i & \mathbf{a}_i \\ \mathbf{a}_i^T & \gamma_{i+1} \end{bmatrix}, \tag{1}$$

with $\mathbf{a}_i = A(1:i, i+1)$ and $\gamma_{i+1} = A(1+i, i+1)$. As a result of this, we will also show that the eigenvalues and eigenvectors of $\hat{A}_{i+1}$ approximate well the dominant eigenvalues and eigenvectors of A_{i+1}.

In this section we describe in detail one step for the iterative procedure of the updating. Let

$$\mathbf{r}_i = U_i^T \mathbf{a}_i, \tag{2}$$

$$\mathbf{q}_i = (I_i - U_i U_i^T)\mathbf{a}_i = \mathbf{a}_i - U_i \mathbf{r}_i, \tag{3}$$

$$\rho_i = \|\mathbf{q}_i\|_2, \tag{4}$$

$$\mathbf{u}_i^{\perp} = \mathbf{q}_i / \rho_i. \tag{5}$$

Remark 2.1. These computations correspond to the Gram–Schmidt orthogonalization [1] of the matrix $[U_n \mid \mathbf{a}]$, and require $4ki$ operations:

$$[U_i \mid \mathbf{a}_i] = \quad [U_i \mid \mathbf{u}_i^{\perp}] \left[\begin{array}{c|c} I_i & \mathbf{r}_i \\ \hline & \rho_i \end{array}\right].$$

To avoid loss of accuracy, in [2] it is suggested to perform the Gram–Schmidt orthogonalization twice, which of course doubles the cost.

Since

$$\mathbf{a}_i = U_i \mathbf{r}_i + \rho_i \mathbf{u}_i^{\perp},$$

then, by (2)–(5), we can write (1) as

$$\hat{A}_{i+1} = \left[\begin{array}{c|c} \tilde{A}_i & \mathbf{a}_i \\ \hline \mathbf{a}_i^T & \gamma_{i+1} \end{array}\right] = \hat{U}_{i+1} \hat{M}_{i+1} \hat{U}_{i+1}^T, \tag{6}$$

where

$$\hat{U}_{i+1} := \left[\begin{array}{c|c|c} \mathbf{u}_i^{\perp} & U_i & \\ \hline & & 1 \end{array}\right], \quad \text{and} \quad \hat{M}_{i+1} := \left[\begin{array}{c|c|c} & & \rho_i \\ \hline & M_i & \mathbf{r}_i \\ \hline \rho_i & \mathbf{r}_i^T & \gamma_{i+1} \end{array}\right]. \tag{7}$$

Let $\hat{M}_{i+1} = \hat{Q}_{i+1} \hat{\Lambda}_{i+1} \hat{Q}_{i+1}^T$ be the spectral decomposition of $\hat{M}_{i+1}$, with $\hat{Q}_{i+1} = [\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_{k+1}, \hat{q}_{k+2}] \in \mathbb{R}^{(k+2)\times(k+2)}$ orthogonal and $\hat{\Lambda}_{i+1} = \operatorname{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_{k+1}, \hat{\lambda}_{k+2})$ with $|\hat{\lambda}_1| \ge |\hat{\lambda}_2| \ge \cdots \ge |\hat{\lambda}_{k+1}| \ge |\hat{\lambda}_{k+2}|$. The best rank–$k$ approximations of $\hat{M}_{i+1}$ and $\hat{A}_{i+1}$ are given, respectively, by

$$\tilde{M}_{i+1} = \sum_{j=1}^{k} \hat{\lambda}_j \hat{q}_j \hat{q}_j^T, \qquad \tilde{A}_{i+1} = \hat{U}_{i+1} \tilde{M}_{i+1} \hat{U}_{i+1}^T.$$

Let $\tilde{V}_{i+1} \in \mathbb{R}^{(k+2)\times(k+2)}$ be the orthogonal matrix such that the last two columns of the product $\hat{V}_{i+1} = \tilde{V}_{i+1} \hat{Q}_{i+1}$ are

$$\hat{V}_{i+1} \mathbf{e}_{i+1}^{(k+2)} = \pm \mathbf{e}_{j_1}^{(k+2)}, \qquad \hat{V}_{i+1} \mathbf{e}_{i+2}^{(k+2)} = \pm \mathbf{e}_{j_2}^{(k+2)},$$

$j_1, j_2 \in \{1, \ldots, i+1, i+2\}$, $j_1 \ne j_2$, where $\mathbf{e}_j^{(k+2)}$, $j = 1, \ldots, k+2$ is the j-th vector of the canonical basis of $\mathbb{R}^{(k+2)}$.

Let $\breve{M}_{i+1} = \hat{V}_{i+1}\hat{M}_{i+1}\hat{V}_{i+1}^T$. Then, for $j \in \{1, 2, \ldots, k, k+1, k+2\}$,

$$\mathbf{e}_{j_1}^{(k+2)^T}\breve{M}_{i+1}\mathbf{e}_j^{(k+2)} = \mathbf{e}_j^{(k+2)^T}\breve{M}_{i+1}\mathbf{e}_{j_1}^{(k+2)} = \begin{cases}\lambda_{k+1}, & j_1 = j,\\ 0, & j_1 \neq j,\end{cases}$$

$$\mathbf{e}_{j_2}^{(k+2)^T}\breve{M}_{i+1}\mathbf{e}_j^{(k+2)} = \mathbf{e}_j^{(k+2)^T}\breve{M}_{i+1}\mathbf{e}_{j_2}^{(k+2)} = \begin{cases}\lambda_{k+2}, & j_1 = j,\\ 0, & j_2 \neq j,\end{cases}$$

i.e., the entries of the rows/columns j_1 and j_2 of $\breve{M}_{i+1}$ are zero but the entries on the main diagonal are equal to λ_{k+1} and λ_{k+2}, respectively. Therefore, the best rank−k approximation of $\hat{A}_{i+1}$ is given by $U_{i+1}M_{i+1}U_{i+1}^T$ where the matrix with orthogonal columns $U_{i+1} \in \mathbb{R}^{(i+1)\times k}$ is obtained by deleting from the product

$$\hat{U}_{i+1}\hat{V}_{i+1}^T \in \mathbb{R}^{(i+1)\times(k+2)} \tag{8}$$

columns j_1 and j_2, and the matrix $M_{i+1} \in \mathbb{R}^{k\times k}$ is obtained from $\breve{M}_{i+1} \in \mathbb{R}^{(k+2)\times(k+2)}$ by removing rows/columns j_1 and j_2. This process of shrinking the matrix is called *deflation*.

Remark 2.2. Instead of computing the product (8), to halve the computation, in [3] it is recommended to factor the matrix U_{i+1} into the product of two orthogonal matrices, $U_{i+1} = U_{i+1}^{(1)}U_{i+1}^{(2)}$, $U_{i+1}^{(1)} \in \mathbb{R}^{(i+1)\times k}$, $U_{i+1}^{(2)} \in \mathbb{R}^{k\times k}$.

The algorithm for tracking the eigenspace corresponding to the k largest eigenvalues in absolute value of a symmetric indefinite matrix can be summarized as follows.

(1) Initialization: compute the best rank−k approximation of A_l, $l > k$ in
the form $\tilde{A}_l = U_l M_l U_l^T$, $U_l \in \mathbb{R}^{l\times k}$ orthogonal and $M_l \in \mathbb{R}^{k\times k}$ symmetric;
`for` $i = l+1 : n$,
(2) compute $\hat{U}_i \in \mathbb{R}^{i\times(k+2)}$ and $\hat{M}_i \in \mathbb{R}^{(k+2)\times(k+2)}$ as in (7);
(3) compute the eigenspace V for the two smallest eigenvalues in absolute value of $\hat{M}_i$;
(4) compute $U_i \in \mathbb{R}^{i\times k}$ and $M_i \in \mathbb{R}^{k\times k}$ deflating the subspace V from $\hat{M}_i$;
`end for`

Of course, to have an efficient procedure of updating it turns out that it is important to efficiently compute (3) and (4), i.e. to compute in an efficient way the eigenvectors corresponding to the 2 eigenvalues λ_{k+1} and λ_{k+2} of $\hat{M}_i$ and to update the matrix M_i in an efficient way from M_{i-1} inheriting its structure.

One could think that diagonal or tridiagonal can be a straightforward choice for the structure of M_i. Although the computation of one of the eigenvalues and corresponding eigenvector of the latter matrices can be done in a fast way, the reduction of M_i in the same form of M_{i-1} requires $O(k^2)$ rotations. Therefore, the updating of the orthogonal factor of the decomposition in (7) requires $O(ik^2)$ floating point operations [4–6]. To reduce the complexity, in this paper we consider M_i with symmetric lower block anti-triangular structure [7]. In fact, if M_{i-1} is lower block anti-triangular in proper form, so is M_i. Moreover, the computation of an eigenvector and the deflation process can be done with $O(k^2)$ complexity to update M_i and $O(ki)$ to update U_i. In the next two subsections we show how this complexity can be achieved exploiting the properties of symmetric anti-triangular matrices. The algorithm for tracking the subspace associated to the largest eigenvalues in absolute values of a symmetric matrix requires a more detailed description of how the structure of M_i is exploited.

2.1. Properties of lower block anti-triangular matrices

Definition 2.1. A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is lower anti-triangular if $A(i, j) = 0$, $i + j \leq n$.

Definition 2.2. A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is said to be block lower anti-triangular if

$$A = \begin{bmatrix} & & Y^T \\ & X & Z^T \\ Y & Z & W \end{bmatrix},$$

with Y anti-triangular and X and W symmetric.

Let $\text{Inertia}(A) = (n_-, n_0, n_+)$. Let $n_1 = \min(n_-, n_+)$, and $n_2 = \max(n_-, n_+) - n_1$.

Definition 2.3. A symmetric block lower anti-triangular matrix $A \in \mathbb{R}^{n\times n}$ is in proper form if

$$A = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & Y^T \\ \mathbf{0} & \mathbf{0} & X & Z^T \\ \mathbf{0} & Y & Z & W \end{bmatrix} \begin{matrix} \}\, n_0 \\ \}\, n_1 \\ \}\, n_2 \\ \}\, n_1 \end{matrix}$$

with $Z \in \mathbb{R}^{n_1\times n_2}$, $W \in \mathbb{R}^{n_1\times n_1}$ symmetric, $Y \in \mathbb{R}^{n_1\times n_1}$ nonsingular lower anti-triangular, $X \in \mathbb{R}^{n_2\times n_2}$ symmetric definite, i.e., $X = \varepsilon LL^T$ with

$$\varepsilon = \begin{cases} 1, & \text{if } n_+ > n_- \\ -1, & \text{if } n_+ < n_- \end{cases}$$

and L lower triangular. Hence, X is symmetric positive definite if $\varepsilon = 1$ and is symmetric negative definite if $\varepsilon = -1$.

If $A \in \mathbb{R}^{n\times n}$ is a nonsingular symmetric block lower anti-triangular matrix in proper form, i.e., $n_0 = 0$, then

$$A = \begin{bmatrix} \mathbf{0} & \mathbf{0} & Y^T \\ \mathbf{0} & X & Z^T \\ Y & Z & W \end{bmatrix}.$$

It can be shown that any symmetric matrix can be transformed into a block anti-triangular form by orthogonal similarity transformations [7].

Theorem 2.1. *Let $A \in \mathbb{R}^{n\times n}$ be a symmetric indefinite matrix with* $\mathrm{Inertia}(A) = (n_-, n_0, n_+)$ *and* $n_1 = \min(n_-, n_+)$, $n_2 = \max(n_-, n_+) - n_1$. *There exists an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ such that $M = Q^TAQ$ is block anti-triangular in proper form,*

$$M = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & Y^T \\ \mathbf{0} & \mathbf{0} & X & Z^T \\ \mathbf{0} & Y & Z & W \end{bmatrix} \begin{matrix} \}\, n_0 \\ \}\, n_1 \\ \}\, n_2 \\ \}\, n_1 \end{matrix}$$

with $Z \in \mathbb{R}^{n_1\times n_2}$, $W \in \mathbb{R}^{n_1\times n_1}$ symmetric, $Y \in \mathbb{R}^{n_1\times n_1}$ nonsingular lower anti-triangular, $X \in \mathbb{R}^{n_2\times n_2}$ symmetric definite, i.e., $X = \varepsilon LL^T$ with

$$\varepsilon = \begin{cases} 1, & \text{if } n_+ > n_- \\ -1, & \text{if } n_+ < n_- \end{cases}$$

and L lower triangular.

In the sequel, without loss of generality, we suppose $\varepsilon = 1$, i.e., the central block X of A positive definite.

2.2. Computation of an eigenpair of a block anti-triangular matrix

We suppose $M \in \mathbb{R}^{(k+2)\times(k+2)}$ nonsingular anti-triangular in proper form with $\mathrm{Inertia}(M) = (k^-, 0, k^+)$, and $k^- + k^+ = k+2$. Let $k_1 = \min(k^-, k^+)$ and $k_2 = \max(k^-, k^+) - k_1$. The smallest eigenvalue λ in absolute value and the corresponding eigenvector $\mathbf{q}$ of

$$M := \hat{M}_{i+1} = \begin{bmatrix} & & Y^T \\ & X & Z^T \\ Y & Z & W \end{bmatrix}, \quad X = LL^T \in \mathbb{R}^{(k_2)\times(k_2)},$$

can be efficiently computed by inverse iteration with zero shift exploiting the block anti-triangular structure of the matrix. Partitioning $\mathbf{x}$ and $\mathbf{y}$ as

$$\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix} \begin{matrix} \}\, k_1 \\ \}\, k_2, \\ \}\, k_1 \end{matrix} \qquad \mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \mathbf{y}_3 \end{bmatrix} \begin{matrix} \}\, k_1 \\ \}\, k_2, \\ \}\, k_1 \end{matrix}$$

a linear system $M\mathbf{x} = \mathbf{y}$ must be solved at each step of inverse iteration. This is reduced to the following steps.

(a) Solve $Y^T\mathbf{x}_3 = \mathbf{y}_1$.
(b) Solve $(LL^T)\mathbf{x}_2 = \mathbf{y}_2 - Z^T\mathbf{x}_3$.
(c) Solve $Y\mathbf{x}_1 = \mathbf{y}_3 - Z\mathbf{x}_2 - W\mathbf{x}_3$.

Due to the anti-triangular structure of Y, the subsystem in (a) is solved with $k_1^2/2$ floating point operations, the two subsystems in (b) are solved with $k_2^2/2 + 2k_1k_2$ floating point operations and the subsystem in (c) is solved with $k_1^2/2 + 2k_1(k_1 + k_2)$ floating point operations. The convergence of the inverse iteration depends on the choice of the initial guess. It turns out that, from many performed numerical experiments, the most efficient choice for the initial vector at the current iteration is one of the two eigenvectors corresponding to the two smallest eigenvalues in absolute value λ_{k+1} and λ_{k+2} discarded at the previous iteration.

2.3. Deflation of a block anti-triangular matrix

Let λ be the smallest eigenvalue in absolute value of $M \in \mathbb{R}^{(k+2)\times(k+2)}$ and $\mathbf{q}$ the corresponding eigenvector. The deflation procedure in case M is singular is trivial (see [7] for details). Without loss of generality, we suppose $k^+ > k^-$. Hence the matrix M has the following block anti-triangular structure,

$$M = \begin{bmatrix} & & Y^T \\ & X & Z^T \\ Y & Z & W \end{bmatrix},$$

with $Y, W \in \mathbb{R}^{k_1\times k_1}$, Y lower anti-triangular and W symmetric, $Z \in \mathbb{R}^{k_2\times k_1}$, $X \in \mathbb{R}^{k_2\times k_2}$ symmetric definite. Without loss of generality, we assume X positive definite with the lower triangular matrix $L \in \mathbb{R}^{k_2\times k_2}$ as Cholesky factor, i.e., $X = LL^T$. Moreover, we consider $k_2 > 2$. The case $k_2 \leq 2$ can be handled in a straightforward way. The process of deflation is divided into 4 steps. The aim is to construct an orthogonal matrix V transforming the eigenvalue problem

$$M\mathbf{q} = \lambda\mathbf{q} \tag{9}$$

into

$$(VMV^T)(V\mathbf{q}) = \lambda(V\mathbf{q}),$$

such that $(V\mathbf{q}) = \pm\mathbf{e}_{k_1}^{(k+2)}$. The entries of the k_1-th row and column of the matrix VMV^T are equal to zero but the entry in position (k_1, k_1) is equal to λ. Therefore, the best rank $k+1$ approximation of M is given by

$$\tilde{V}\tilde{M}\tilde{V}^T,$$

with $\hat{V} = V(:, [1 : k_1 - 1, k_1 + 1 : k+2]) \in \mathbb{R}^{(k+2)\times(k+1)}$, $\hat{M} = M([1 : k_1 - 1, k_1 + 1 : k+2], [1 : k_1 - 1, k_1 + 1 : k+2]) \in \mathbb{R}^{(k+1)\times(k+1)}$, i.e., $\hat{M}$ is obtained from M removing the k_1-th row and column.

Let $M_0 := M$, $\mathbf{q}_0 := \mathbf{q}$ and $V := I_{k+2}$.

2.4. First step

At the iteration j, $j = 1, \ldots, k_1 - 1$, of this step, the rows j and $j+1$ of $\mathbf{q}$ are modified by the multiplication of a Givens rotation $\tilde{G}_j$ determined such that

$$\tilde{G}_j\mathbf{q}(j : j+1) = \begin{bmatrix} 0 \\ \sqrt{\mathbf{q}(j)^2 + \mathbf{q}(j+1)^2} \end{bmatrix}.$$

Let

$$\tilde{G}^{(j)} = \begin{bmatrix} I_{j-1} & & \\ & \tilde{G}_j & \\ & & I_{k-j+1} \end{bmatrix}.$$

Define

$$\tilde{M} := \tilde{G}^{(j)}M\tilde{G}^{(j)^T}, \qquad \tilde{\mathbf{q}} := \tilde{G}^{(j)}\mathbf{q}, \qquad V := V\tilde{G}^{(j)^T}.$$

The matrix $\tilde{M}$ differs from a block anti-triangular matrix for a bulge in position $(j, n-j)$ and, symmetrically, in position $(n-j, j)$. Moreover, the j-th entry of $\tilde{\mathbf{q}}$ is 0. To remove the bulge and restore the anti-triangular structure in $\tilde{M}$, another Givens rotation $\hat{G}_j$ is considered such that

$$\tilde{M}(j, k+2-j : k-j+1)\hat{G}_j^T = \left[0, \|\tilde{M}(j, k-j+2 : k-j+1)\|_2\right].$$

Let

$$\hat{G}^{(j)} = \begin{bmatrix} I_{j-1} & & \\ & \hat{G}_j & \\ & & I_{k-j+1} \end{bmatrix}$$

and define

$$M := \hat{G}^{(j)}\tilde{M}\hat{G}^{(j)^T}, \qquad \mathbf{q} := \hat{G}^{(j)}\tilde{\mathbf{q}}, \qquad V = V\hat{G}^{(j)^T}.$$

Hence, (9) is transformed into the following eigenvalue problem

$$(VM_0V^T)(V\mathbf{q}_0) = \lambda(V\mathbf{q}_0). \tag{10}$$

The eigenvector $\mathbf{q}$ has the first j entries equal to zero. One can easily prove by induction that also the last j entries, i.e., the entries $k+3-l$, $l = 1, \ldots, j$, are zero. This step, for a matrix M with $k_1 = 3$ and $k_2 = 5$, is graphically depicted in Fig. 1.

Computational complexity. Due to the symmetric block anti-triangular structure of M, at iteration j of this step, $6(k+2)$ and $12j$ floating point operations are required to update M and V, respectively. Therefore the first step needs $6k_1(k+2) + 6k_1^2$ floating point operations.

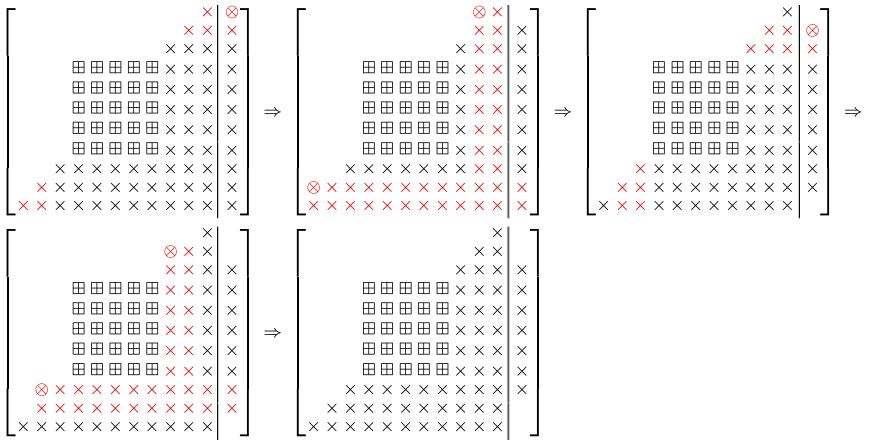

Fig. 1. First step of the algorithm. Graphical representation of the application of the sequence of $k_1 - 1$ Givens transformations to the augmented matrix $[M|q]$. The entries to be annihilated are denoted by $\otimes$ and the entries modified by the multiplication are in red. The entries of the positive definite central submatrix X are denoted by the symbol $\boxplus$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

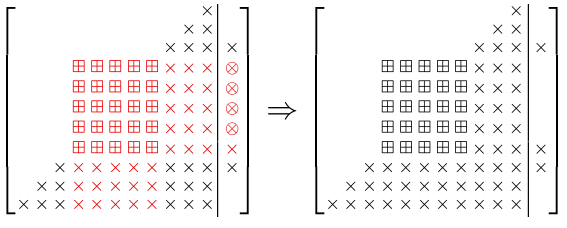

Fig. 2. Second step of the algorithm. Graphical representation of the effect of the multiplication of the sequence of $k_2 - 1$ Givens rotations on the augmented matrix $[M|q]$.

2.5. Second step

Let $\tilde{k}_1 = k_1 - 1$. At the iteration j, $j = 1, \ldots, k_2 - 1$, of this step, the rows $k_1 + j$ and $k_1 + j + 1$ of $\mathbf{q}$ are modified by the multiplication of a Givens rotation $\tilde{G}_{\tilde{k}_1+j}$ determined such that

$$\tilde{G}_{\tilde{k}_1+j}\mathbf{q}(k_1 + j : k_1 + j + 1) = \begin{bmatrix} 0 \\ \sqrt{\mathbf{q}(k_1 + j)^2 + \mathbf{q}(k_1 + j + 1)^2} \end{bmatrix}.$$

Let

$$\tilde{G}^{(\tilde{k}_1+j)} = \begin{bmatrix} I_{\tilde{k}_1+j} & & \\ & \tilde{G}_{\tilde{k}_1+j} & \\ & & I_{k-\tilde{k}_1-j} \end{bmatrix}.$$

Define

$$M := \tilde{G}^{(\tilde{k}_1+j)} M \tilde{G}^{(\tilde{k}_1+j)^T}, \tag{11}$$

$$\mathbf{q} := \tilde{G}^{(\tilde{k}_1+j)}\mathbf{q},$$

$$V := V\tilde{G}^{(\tilde{k}_1+j)^T}. \tag{12}$$

The effect of the whole second step is graphically depicted in Fig. 2. At the j-th iteration of this step, the similarity transformation (11) modifies the lower triangular structure of the Cholesky factor L of the central block X of M introducing a bulge in position $(j, j + 1)$ of L. To restore the lower triangular structure, L must be multiplied to the right by an "inner" Givens rotation $\check{G}_j \in \mathbb{R}^{k_2 \times k_2}$, acting on columns j and $j + 1$ such that $L := L\check{G}_j$ has the entry $(j, j + 1)$ annihilated. This is graphically depicted in Fig. 3.

Computational complexity. At iteration j of this step, (11) and (12) must be computed, requiring both $6k_1 + 6j$ floating point operations. Moreover, to restore the lower triangular structure in L, $6(k_2 - j)$ floating point operations are needed. Therefore the second step needs $12k_1k_2 + 6k_2^2$ floating point operations.

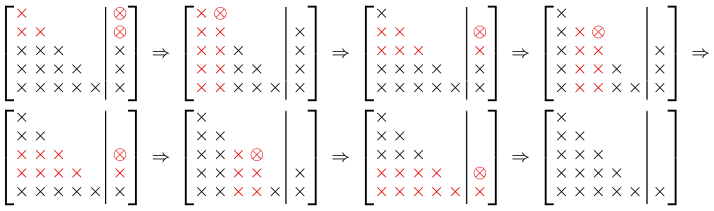

Fig. 3. Second step of the algorithm. For the sake of brevity, only the influence of the Givens rotations on the Cholesky factor L of X and the corresponding entries of the eigenvector is depicted. To preserve the Cholesky structure, each multiplication by an outer Givens rotation $\tilde{G}^{(\tilde{k}_1+j)}$, introducing a bulge in the lower triangular structure of L, is followed by a multiplication by an inner Givens rotation $\check{G}_j$ removing the bulge.

2.6. Third step

In this step, first a Givens rotation $\tilde{G}_{k_1+k_2-1} \in \mathbb{R}^{2\times 2}$ is determined such that

$$\tilde{G}_{k_1+k_2-1}\mathbf{q}(k_1+k_2 : k_1+k_2+1) = \begin{bmatrix} 0 \\ \sqrt{\mathbf{q}(k_1+k_2)^2 + \mathbf{q}(k_1+k_2+1)^2} \end{bmatrix}.$$

Let

$$\tilde{G}^{(k_1+k_2-1)} = \begin{bmatrix} I_{k_1+k_2-1} & & \\ & \tilde{G}_{k_1+k_2-1} & \\ & & I_{k_1-1} \end{bmatrix}.$$

Define

$$\begin{aligned} M &:= \tilde{G}^{(k_1+k_2-1)} M \tilde{G}^{(k_1+k_2-1)^T}, \\ \mathbf{q} &:= \tilde{G}^{(k_1+k_2-1)}\mathbf{q}\, V := V\tilde{G}^{(k_1+k_2-1)^T}. \end{aligned} \tag{13}$$

Since

$$M\mathbf{q} = \lambda\mathbf{q}, \tag{14}$$

it turns out that $M(k_1+1 : k_1+k_2-1, k_1+k_2) = \mathbf{0}$ and, symmetrically, $M(k_1+k_2, k_1+1 : k_1+k_2-1) = \mathbf{0}$. Due to the fact that only the k_1-th and (k_1+k_2)-th entries of $\mathbf{q}$ differ from zero, from (14) we have

$$M(k_1+1 : k_1+k_2-1, [k_1, k_1+k_2])\mathbf{q}([k_1, k_1+k_2]) = \mathbf{0}.$$

Hence, $M(k_1+1 : k_1+k_2-1, k_1+k_2) = \mathbf{0}$ since $M(k_1+1 : k_1+k_2-1, k_1) = \mathbf{0}$. This part of the third step is graphically depicted in the first transformation in Fig. 4. To end this step, another Givens rotation, acting on the k_1-th and (k_1+k_2)-th entries of $\mathbf{q}$ annihilating the entry (k_1+k_2), must be applied. Let $\tilde{G}_{k_1+k_2} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \in \mathbb{R}^{2\times 2}$ be a Givens rotation such that

$$\tilde{G}_{k_1+k_2}\mathbf{q}([k_1, k_1+k_2]) = \begin{bmatrix} 0 \\ \sqrt{\mathbf{q}(k_1)^2 + \mathbf{q}(k_1+k_2)^2} \end{bmatrix}.$$

Let $\check{M}$ be the 2×2 symmetric anti-triangular matrix formed intersecting the k_1-th and k_1+k_2-th rows and columns of M, i.e.,

$$\check{M} := \begin{bmatrix} 0 & M(k_1, k_1+k_2) \\ M(k_1+k_2, k_1) & M(k_1+k_2, k_1+k_2) \end{bmatrix}.$$

We observe that $\tilde{G}_{k_1+k_2}$ diagonalizes $\check{M}$, i.e.,

$$\tilde{G}_{k_1+k_2-1}\check{M}\tilde{G}_{k_1+k_2-1}^T = \begin{bmatrix} \lambda & \\ & \gamma_1 \end{bmatrix},$$

with $\lambda\gamma_1 < 0$. Let

$$\tilde{G}^{(k_1+k_2)} = \begin{bmatrix} I_{k_1-1} & & & & \\ & c & & s & \\ & & I_{k_2-1} & & \\ & -s & & c & \\ & & & & I_{k_1} \end{bmatrix}.$$

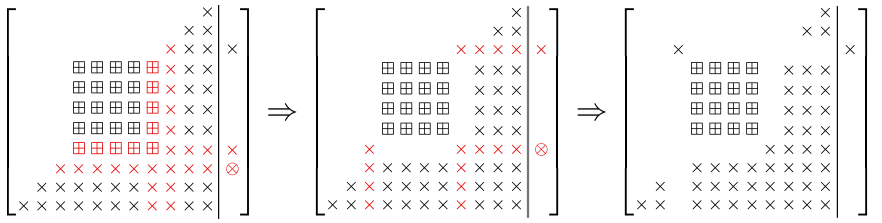

Fig. 4. Third step of the algorithm.

Let

$$\begin{aligned} M &:= \tilde{G}^{(k_1+k_2)} M \tilde{G}^{(k_1+k_2)^T}, \\ \mathbf{q} &:= \tilde{G}^{(k_1+k_2)} \mathbf{q} \equiv \pm \mathbf{e}_{k_1}^{(k+2)}, \\ V &:= V \tilde{G}^{(k_1+k_2)^T}. \end{aligned} \tag{15}$$

We observe that in (15), $M(k_1+1 : k_1+k_2-1, k_1+k_2) = \mathbf{0}$ and, symmetrically, $M(k_1+k_2, k_1+1 : k_1+k_2-1) = \mathbf{0}$. Moreover, the number of floating point operations of this step depends linearly on k_1 and k_2 and it is therefore negligible.

2.7. Step 4

In this step, $\hat{M}$ is constructed removing the row and column k_1 from M. Hence $\hat{M}$ has the following symmetric block anti-triangular structure,

$$\begin{bmatrix} \mathbf{0} & \mathbf{0} & \hat{Y}^T \\ \mathbf{0} & \hat{X} & \hat{Z}^T \\ \hat{Y} & \hat{Z} & \hat{W} \end{bmatrix} \begin{matrix} \} k_1 - 1 \\ \} k_2 + 1, \\ \} k_1 - 1 \end{matrix} \quad \hat{X} = \left[\begin{array}{cc|c} LL^T & \mathbf{0} & \mathbf{t} \\ \mathbf{0}^T & \gamma_1 & \\ \hline \mathbf{t}^T & & \gamma_2 \end{array}\right]. \tag{16}$$

Moreover, $\tilde{V}$ is constructed removing the row and column k_1 from V. Depending on the sign of λ, we have to distinguish the following 2 cases.

Case 1: $\lambda < 0$. In this case, $\text{Inertia}(\hat{M}) = (k_- - 1, 0, k_+)$. Hence, the central block $\hat{X} \in \mathbb{R}^{(k_2+1)\times(k_2+1)}$ is symmetric positive definite. We need only to update the Cholesky factor $\hat{L}$ of $\hat{X}$, i.e., compute the last two rows of $\hat{L}$, since $\hat{L}(1 : k_2-1, 1 : k_2-1) = L(1 : k_2-1, 1 : k_2-1)$.

$$\begin{aligned} &\hat{L}(k_2, 1 : k_2-1) = \mathbf{0}; \qquad \hat{L}(k_2, 1 : k_2) = \sqrt{\hat{X}(k_2, k_2)}; \\ &\text{solve } \hat{L}(1 : k_2, 1 : k_2)(\hat{L}(k_2+1, 1 : k_2))^T = \hat{X}(1 : k_2, k_2+1); \\ &\hat{L}(k_2+1, k_2+1) = \hat{X}(k_2+1, k_2+1)^2 - \mathbf{l}^T\mathbf{l}, \end{aligned} \tag{17}$$

with $\mathbf{l} = \hat{L}(k_2+1, 1 : k_2)^T$. The solution of the linear system (17) requires k_2^2 floating point operations.

Case 2: $\lambda > 0$. In this case, $\text{Inertia}(\hat{M}) = (k^-, 0, k^+ - 1)$. Although $\hat{M}$ is symmetric block anti-triangular, the central block $\hat{X}$ is indefinite. Since $\text{Inertia}(\hat{X}) = (1, 0, k_2)$, we first transform $\hat{X}$ into a block anti-triangular submatrix in proper form. Let us decompose $L \in \mathbb{R}^{(k_2-1)\times(k_2-1)}$ as

$$L = \begin{bmatrix} L_1 & \\ \mathbf{l}_1^T & \beta_1 \end{bmatrix},$$

with $L_1 \in \mathbb{R}^{(k_2-2)\times(k_2-2)}$, $\mathbf{l}_1 \in \mathbb{R}^{k_2-2}$, $\beta_1 \in \mathbb{R}$. Let $\gamma_1 = \hat{X}(k_2, k_2) < 0$. Therefore

$$\hat{X}(1 : k_2, 1 : k_2) = \begin{bmatrix} L_1 \\ \mathbf{l}_1^T \\ \mathbf{0}^T \end{bmatrix} \begin{bmatrix} L_1^T & \mathbf{l}_1 & \mathbf{0} \end{bmatrix} + \left[\begin{array}{c|c|c} & & \\ \hline & \beta_1^2 & \\ \hline & & \gamma_1 \end{array}\right].$$

Let $\hat{X}_0 := X$. Let $Q_2 \in \mathbb{R}^{2\times 2}$ be the orthogonal matrix such that

$$Q_2 \begin{bmatrix} \beta_1^2 & \\ & \gamma_1 \end{bmatrix} Q_2^T = \begin{bmatrix} 0 & \xi_1 \\ \xi_1 & \xi_2 \end{bmatrix}.$$

Let

$$\begin{bmatrix} \mathbf{l}_2^T \\ \mathbf{l}_3^T \end{bmatrix} = Q_2 \begin{bmatrix} \mathbf{l}_1^T \\ \mathbf{0}^T \end{bmatrix}.$$

Then

$$\hat{X}(1:k_2,1:k_2) := \begin{bmatrix} I_{k_2-2} & \\ & Q_2 \end{bmatrix} \hat{X}(1:k_2,1:k_2) \begin{bmatrix} I_{k_2-2} & \\ & Q_2^T \end{bmatrix} = \begin{bmatrix} L_1 \\ \mathbf{l}_2^T \\ \mathbf{l}_3^T \end{bmatrix} \begin{bmatrix} L_1^T & \mathbf{l}_2 & \mathbf{l}_3 \end{bmatrix} + \left[\begin{array}{c|cc} & & \\ \hline & 0 & \xi_1 \\ & \xi_1 & \xi_2 \end{array}\right].$$

Let $\Gamma = G_{k_2-2}G_{k_2-3}\cdots G_1$, where $G_i \in \mathbb{R}^{(k_2-1)\times(k_2-1)}$, $i = 1,\ldots,k_2-2$ is the sequence of Givens rotations such that

$$\begin{bmatrix} \mathbf{0} \\ L_2 \end{bmatrix} = \Gamma \begin{bmatrix} L_1 \\ \mathbf{l}_2^T \end{bmatrix}, \tag{18}$$

with $L_2 \in \mathbb{R}^{(k_2-2)\times(k_2-2)}$ lower triangular. Then

$$\hat{X}(1:k_2,1:k_2) = \begin{bmatrix} \Gamma & \\ & 1 \end{bmatrix} \hat{X}(1:k_2,1:k_2) \begin{bmatrix} \Gamma^T & \\ & 1 \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & L_2L_2^T & L_2\mathbf{l}_3 \\ \mathbf{0} & \mathbf{l}_3^TL_2^T & \mathbf{l}_3^T\mathbf{l}_3 \end{bmatrix} + \left[\begin{array}{cc|c} & & \mathbf{z} \\ & & \\ \hline \mathbf{z}^T & & \xi_2 \end{array}\right],$$

$\mathbf{z} = \xi_1\Gamma \mathrm{e}_{k_2-1}^{(k_2-1)}$. Let $\tilde{\mathbf{z}} = \begin{bmatrix} \mathbf{0} \\ L_2\mathbf{l}_3 \end{bmatrix} + \mathbf{z}$, $\hat{\gamma}_1 = \mathbf{l}_3^T\mathbf{l}_3 + \xi_2$. Then

$$\hat{X} = \left[\begin{array}{cc|c|c} 0 & \mathbf{0} & \tilde{\mathbf{z}} & \\ \mathbf{0}^T & L_2L_2^T & & \mathbf{t} \\ \hline \multicolumn{2}{c|}{\tilde{\mathbf{z}}^T} & \hat{\gamma}_1 & \\ \hline \multicolumn{3}{c|}{\mathbf{t}^T} & \gamma_2 \end{array}\right].$$

Let

$$\hat{\Gamma} := \begin{bmatrix} I_{k_1-1} & & \\ & \Gamma & \\ & & I_{k_1+1} \end{bmatrix} \begin{bmatrix} I_{k_1+k2-3} & & \\ & Q_2 & \\ & & I_{k_1+1} \end{bmatrix}.$$

Then

$$\hat{M} := \hat{\Gamma}\hat{M}\hat{\Gamma}^T \quad \text{and} \quad V := V\hat{\Gamma}^T.$$

To reduce $\hat{M}$ in proper form, we construct the Givens matrix $\hat{Q}_3 = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$ such that

$$\hat{Q}_3 \begin{bmatrix} \mathbf{t}(1) \\ \tilde{\mathbf{z}}(1) \end{bmatrix} = \begin{bmatrix} 0 \\ \sqrt{\mathbf{t}(1)^2 + \tilde{\mathbf{z}}(1)^2} \end{bmatrix}.$$

Let

$$\tilde{Q}_3 = \begin{bmatrix} I_{k_1-1} & \\ & \hat{Q}_3 \end{bmatrix} \quad \text{and} \quad Q_3 = \begin{bmatrix} I_{k_1+k_2-2} & & \\ & \hat{Q}_3 & \\ & & I_{k_1-1} \end{bmatrix}.$$

Then

$$\hat{M} := Q_3\hat{M}Q_3^T$$

is a block lower anti-triangular matrix in proper form,

$$\hat{M} = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \hat{Y}^T \\ \mathbf{0} & \hat{X} & \hat{Z}^T \\ \hat{Y} & \hat{Z} & \hat{W} \end{bmatrix} \begin{matrix} \} k_1 \\ \} k_2 - 1 \\ \} k_1. \end{matrix}$$

Moreover, let $V := VQ_3^T$. We observe that

$$\hat{X} = \begin{bmatrix} L_2L_2^T & \hat{X}(1:k_2-1,k_2-1) \\ \hat{X}(k_2-1,1:k_2-1) & \hat{X}(k_2-1,k_2-1) \end{bmatrix}.$$

Hence to compute the Cholesky factor $\hat{L}$ of $\hat{X}$ we need to compute only its last row, since $\hat{L}(1:k_2-1,1:k_2-1) = L_2$,

$$\begin{aligned} &\hat{L}(1:k_2-,1:k_2-1) = L_2; \\ &\text{solve } \hat{L}(1:k_2-1,1:k_2-1)(\hat{L}(k_2,1:k_2-1))^T = \hat{X}(1:k_2-1,k_2); \\ &\hat{L}(k_2,k_2) = \hat{X}(k_2,k_2)^2 - \mathbf{l}_4^T\mathbf{l}_4, \end{aligned} \tag{19}$$

with $\mathbf{l}_4 = \hat{L}(k_2,1:k_2-1)$. This is graphically depicted in the last transformation of Fig. 5.

Computational complexity. The required number of floating point operations to update $\hat{M}$ and V are $3k_2^2 + 6k_1k_2$ and $12k_1k_2 + 6k_2^2$, respectively.

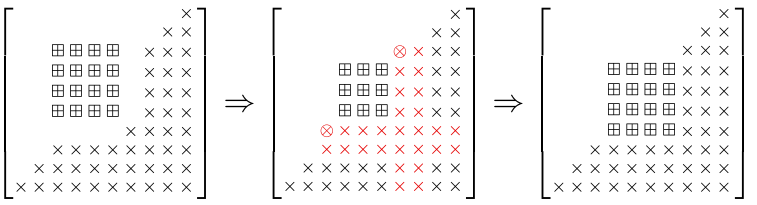

Fig. 5. Fourth step of the algorithm. Transformation of the block anti-triangular matrix of Case 2 in proper form.

3. Accuracy bounds

In this section we provide some bounds on the error of the low rank approximation of the symmetric matrix. For this we study the local approximation errors and show that these can be used to provide estimates for the global error at the end of the algorithm. Let $A_n \in \mathbb{R}^{n\times n}$ be a symmetric matrix with eigenvalue decomposition

$$A_n = V_n \Lambda_n V_n^T,$$

with $\Lambda_n = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, where we have ordered the eigenvalues according to their non-increasing amplitude :

$$|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_n| \geq 0$$

since these are the ordered singular values of A_n. Let A_i be any $i \times i$ principal submatrix of order i with eigenvalue decomposition

$$A_i = V_i \Lambda_i^{(i)} V_i^T,$$

where $\Lambda_i^{(i)} = \mathrm{diag}(\lambda_1^{(i)}, \ldots, \lambda_i^{(i)})$, and $|\lambda_1^{(i)}| \geq |\lambda_2^{(i)}| \geq \cdots \geq |\lambda_i^{(i)}| \geq 0$.

It follows from the interlacing properties of singular values, that

$$|\lambda_j| \geq |\lambda_j^{(i+1)}| \geq |\lambda_j^{(i)}| \quad j = 1, \ldots, i, \tag{20}$$

which shows that each singular value $|\lambda_j^{(i)}|$ is a non-decreasing function of i.

In the updating scheme, we approximated A_i by a rank k approximation

$$A_i \approx \tilde{A}_i = U_i M_i U_i^T, \quad U_i^T U_i = I_k, M_i = M_i^T$$

which was obtained recursively for $i = l+1, \ldots, n$ (with $l > k$). The first approximation $\tilde{A}_l$ is assumed to be an optimal rank k approximation of A_l, i.e. $E_l := A_l - \tilde{A}_l$ has non-trivial singular values $|\lambda_{k+1}^{(l)}|, \ldots, |\lambda_l^{(l)}|$. All subsequent approximations were obtained by solving a local minimization problem at each iteration step n, using the bordered matrix problem

$$\min \left\| \left[\begin{array}{c|c} U_i M_i U_i^T & \mathbf{a}_i \\ \hline \mathbf{a}_i^T & \gamma_{i+1} \end{array}\right] - U_{i+1} M_{i+1} U_{i+1}^T \right\|_F^2, \tag{21}$$

such that $M_{i+1} = M_{i+1}^T$ and $U_{i+1}^T U_{i+1} = I_k$, where $\mathbf{a}_i$, γ_{i+1} are the elements of the bordered matrix

$$A_{i+1} = \left[\begin{array}{c|c} A_i & \mathbf{a}_i \\ \hline \mathbf{a}_i^T & \gamma_{i+1} \end{array}\right].$$

We indicate here that (21) always has a unique solution in the Frobenius norm and that it also minimizes the 2 norm of (21).

We now try to bound the error matrix $E_i := A_i - \tilde{A}_i$ at each step, both in the 2-norm $\|E_i\|_2$ and the Frobenius norm $\|E_i\|_F$. For this, we use the updating formulas for $\tilde{A}_{i+1}$, which is a rank 2 correction to $\hat{A}_{i+1}$:

$$\tilde{A}_{i+1} = \hat{A}_{i+1} - W_{i+1} \Delta_{i+1} W_{i+1}^T, \qquad \hat{A}_i := \left[\begin{array}{c|c} \tilde{A}_i & \mathbf{a}_i \\ \hline \mathbf{a}_i^T & \gamma_{i+1} \end{array}\right], \qquad \Delta_{i+1} := \begin{bmatrix} \hat{\lambda}_{k+1}^{(i)} & 0 \\ 0 & \hat{\lambda}_{k+2}^{(i)} \end{bmatrix}$$

with $\hat{\lambda}_{k+1}^{(i)}$ and $\hat{\lambda}_{k+2}^{(i)}$, the two deflated eigenvalues of $\hat{A}_i$ and $W := \left[w_{k+1}^{(i)}\ w_{k+2}^{(i)}\right]$, the matrix of corresponding eigenvectors. Moreover, we have

$$A_{i+1} - \tilde{A}_{i+1} = \left[\begin{array}{c|c} A_i - \tilde{A}_i & \mathbf{0} \\ \hline \mathbf{0}^T & 0 \end{array}\right] + W_{i+1} \Delta_{i+1} W_{i+1}^T.$$

Hence, it follows that

$$\|A_{i+1} - \tilde{A}_{i+1}\|_2 \leq \|A_i - \tilde{A}_i\|_2 + |\hat{\lambda}_{k+1}^{(i)}|,$$
$$\|A_{i+1} - \tilde{A}_{i+1}\|_F^2 \leq \|A_i - \tilde{A}_i\|_F^2 + (\hat{\lambda}_{k+1}^{(i)})^2 + (\hat{\lambda}_{k+2}^{(i)})^2.$$

If we start with $A_{\tilde{i}} = \tilde{A}_{\tilde{i}} + E_{\tilde{i}}$, then by induction we obtain at step i

$$A_i - \tilde{A}_i = \hat{E}_{\tilde{i}} + W \Delta W^T,$$

where Δ is a block-diagonal matrix of order $2(i-l)$, containing the diagonal blocks Δ_i, $\hat{E}_l$ is E_l padded with zeros, and W contains the successive block columns W_i, also padded with zeros in order to have matching dimensions. It immediately follows that

$$\|A_n - \tilde{A}_n\|_F^2 \le \eta_n := \sum_{i=k+1}^{l} {\lambda_i^{(l)}}^2 + \sum_{i=l+1}^{n} (\hat{\lambda}_{k+1}^{(i)})^2 + \sum_{i=l+1}^{n} (\hat{\lambda}_{k+2}^{(i)})^2, \tag{22}$$

$$\|A_n - \tilde{A}_n\|_2 \le \zeta_n := |\lambda_{k+1}^{(l)}| + \sum_{i=l+1}^{n} |\hat{\lambda}_{k+1}^{(i)}|. \tag{23}$$

Although we could not prove this, we observed that in practice $|\hat{\lambda}_{k+1}^{(i)}| \le |\lambda_{k+1}^{(i)}|$ and since it follows from the interlacing inequalities that $|\lambda_{k+1}^{(i)}| \le |\lambda_{k+1}|$ we finally obtain

$$\sum_{i=k+1}^{n} \lambda_i^2 \le \|A_n - \tilde{A}_n\|_F^2 \lessapprox 2(n-k)\lambda_{k+1}^2.$$

If, moreover, the vectors in W are nearly orthogonal to each other then one would also have

$$|\lambda_{k+1}| \le \|A_n - \tilde{A}_n\|_2 \lessapprox c|\lambda_{k+1}|,$$

with $c \approx 1$. We will verify in the examples of the next section, that this is nearly satisfied, but there is of course no guarantee that this last bound always holds. The fact that $c \approx 1$ implies that the obtained bound is globally optimal, while we constructed only locally optimal approximations. We expect that the explanation ought to be found in the randomness of the bordering vectors.

4. Numerical results

Some numerical experiments, showing the properties of the proposed algorithm, are reported in this section. In particular, it is shown that the numerical results agree with the empirical bound of the previous section. The experiments are carried out in `matlab`.

Example 4.1. In this example, we examine the behavior of the proposed algorithm applied to the indefinite symmetric matrices $A := A(\alpha)$, depending on the parameter α, constructed as follows.

Let $n = 100$, $d = [-10*\texttt{ones}(10,1); 8*\texttt{ones}(10,1); \alpha*\texttt{randn}(80,1)] + \alpha*\texttt{randn}(100,1)$, and $A = Q\,\texttt{diag}(d(P))Q^T$, with Q a random orthogonal matrix of order 100, P a random permutation of the indices of the vector d and $\alpha = 10^{-i}$, $i = 0, 1, \ldots, 5$.

Therefore, the matrices A are nonsingular, with 10 eigenvalues clustered around -10, and 10 ones around 8. The size of the initialization problem is $l = 30$ and the rank chosen for the approximation is $k = 20$, i.e., at each iteration of the algorithm, the subspace corresponding to the largest 20 eigenvalues in absolute value is tracked. The eigenvalues of the matrix A and the eigenvalues of the matrix $\tilde{A}_n$, for $\alpha = 1$, are depicted in Fig. 6. The left (asterisk) and the right (circle) hand side of the bound (22), for $l = 31, 32, \ldots, 100$, are reported in Fig. 7. We have also run the algorithm for $\alpha = 10^{-i}$, $i = 0, 1, \ldots, 5$, and the size of the initialization problem l equal to 50 and rank of the approximation k equal to 40. Let us denote by $V_{30,20}^{(20)}$ and by $V_{50,40}^{(20)}$, the subspaces spanned by the eigenvectors corresponding to the 20 largest eigenvalues in absolute value of the matrix $\tilde{A}_n$ computed by the proposed algorithm with the size of the initialization problem l equal to 30 and 50, and the rank k (i.e. the order of the matrix M) equal to 20 and 40, respectively. Moreover, let $V^{(20)}$ be the subspace spanned by the eigenvectors corresponding to the 20 largest eigenvalues in absolute value of A computed by the matlab function `eigs`. In Table 1, the angles between the subspaces V and $V_{30,20}^{(20)}$ and by $V_{50,40}^{(20)}$ for different values of α are reported. The angles between the subspaces seems to depend quadratically on the parameter α.

Example 4.2. Let

$$F(i,j) = \sum_{k=1}^{3} (-1)^k \exp\left(-\frac{(i-\mu_k)^2 + (j-\mu_k)^2}{2\sigma_k}\right), \quad i,j = 1, \ldots, 100,$$

with

$$\mu = \begin{bmatrix} 4 & 18 & 76 \end{bmatrix}, \qquad \sigma = \begin{bmatrix} 10 & 20 & 5 \end{bmatrix}.$$

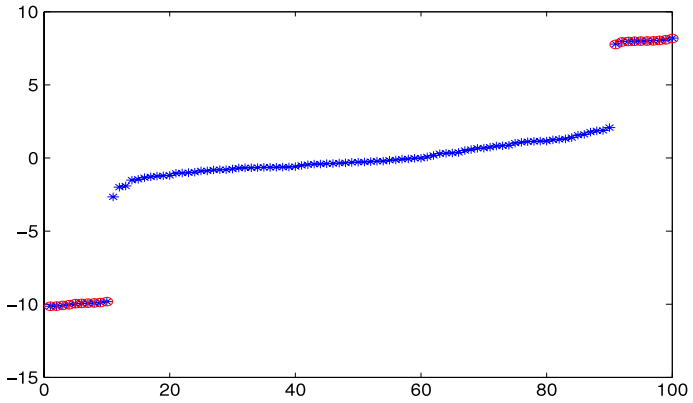

Fig. 6. Plot of the eigenvalues of the matrix A_n, with $\alpha = 1$, (asterisk) and of those of the matrix $\tilde{A}_n$ (circle).

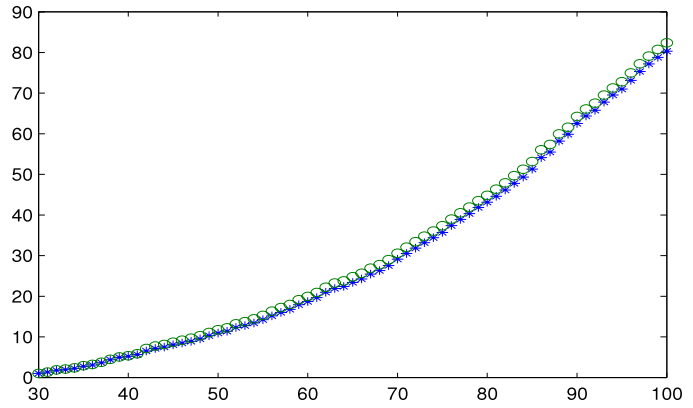

Fig. 7. Plot of $\|A_k - \tilde{A}_k\|_F$ (asterisk) and η_k (circle) of Example 4.1.

Table 1
Angles between the subspaces spanned by the eigenvectors corresponding to the largest 20 eigenvalues of A computed by the function `eigs` of `matlab` and the corresponding ones of UMU^T computed by the proposed algorithm for different values of α.

α	$\angle(V^{(20)}, V^{(20)}_{30,20})$	$\angle(V^{(20)}, V^{(20)}_{50,40})$
10^0	1.5683e−002	7.1443e−003
10^{-1}	4.4014e−004	1.4602e−004
10^{-2}	2.2637e−006	1.2077e−006
10^{-3}	3.6738e−008	1.0810e−008
10^{-4}	2.7103e−010	1.0118e−010
10^{-5}	8.5140e−012	4.8410e−012

Hence, F is a rank 3 matrix. Let $F = Q\Lambda Q^T$ be its spectral decomposition and let $\tilde{\Delta} \in \mathbb{R}^{100\times 100}$ be a matrix of random numbers generated by the `matlab` function `randn`, and define $\Delta = (\tilde{\Delta} + \tilde{\Delta}^T)/\|\tilde{\Delta} + \tilde{\Delta}^T\|_2$. For this example, the considered symmetric indefinite matrix is (Fig. 8)

$$A_n = F + \varepsilon\Delta$$

with $n = 100$ and $\varepsilon = 1.0\text{e}{-3}$.

The left (asterisk) and the right (circle) hand side of the bound (22), for $l = 4, 5, \ldots, 100$, are reported in Fig. 9. In Table 2 the largest three eigenvalues in absolute value of the matrix A computed by the function `eigs` of `matlab` and the corresponding ones of the matrix $\tilde{A}_n$ computed by the proposed algorithm with $l = 10$ and rank $k = 3$. The angle between $V^{(3)}$ be the subspace spanned by the eigenvectors corresponding to the 3 largest eigenvalues in absolute value of A_n computed by the matlab function `eigs` and the subspace $V^{(3)}_{10,3}$, the subspace spanned by the eigenvectors corresponding to the 3 largest eigenvalues in absolute value of the matrix $\tilde{A}_n$ computed by the proposed algorithm with $l = 10$ and rank $k = 3$, is 4.8878e−007.

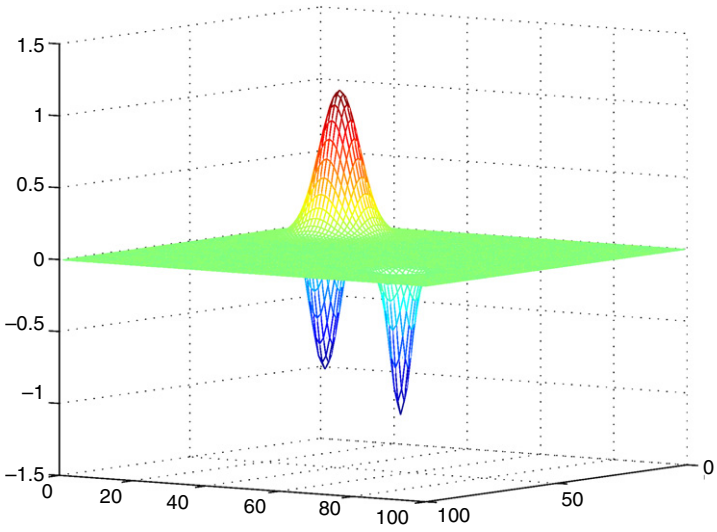

Fig. 8. Plot of the entries of the matrix A_n of Example 4.2.

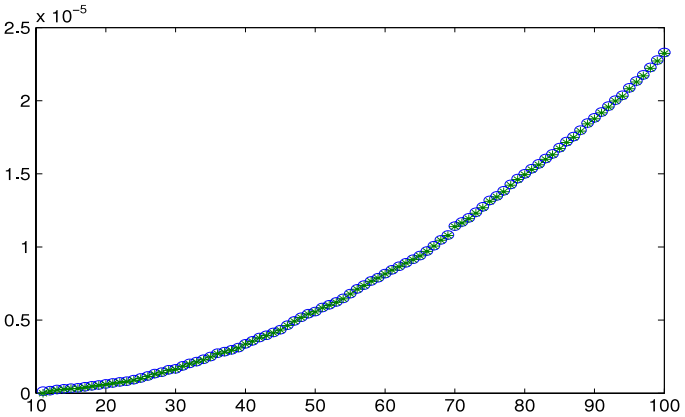

Fig. 9. Plot of $\|A_k - \tilde{A}_k\|_F$ (asterisk) and η_k (circle) of Example 4.2.

Table 2
First three eigenvalues of the matrix A_n (Example 4.2) computed by the function `eigs` of `matlab` and the corresponding ones of the matrix $\tilde{A}_n$ by the proposed algorithm.

i	$\lambda_i(A_n)$	$\lambda_i(\tilde{A}_n)$
1	7.922052200064504e+000	7.922052200062411e+000
2	−5.279522842849688e+000	−5.279522842849557e+000
3	−3.963518913702159e+000	−3.963518920320980e+000

Example 4.3. The matrix A considered in this example is the real part of the complex symmetric matrix called QC324, obtained from the `Matrix Market` [8], modeling H_2^+ in an Electromagnetic Field, and depicted in Fig. 10. Its order is $n = 324$ and it has 211 negative and 113 positive eigenvalues, respectively. The size of the initialization problem is 60 and the rank chosen for the approximation is 40, i.e., at each iteration of the algorithm, the subspace corresponding to the largest 40 eigenvalues in absolute value is tracked. The eigenvalues of the matrix A_n and those of the matrix $\tilde{A}_n$ are depicted in Fig. 11. The left (asterisk) and the right (circle) hand side of the bound (22), for $l = 61, 62, \ldots, 324$, are reported in Fig. 12.

In Fig. 13 we show the inertia of the matrices $M_i \in \mathbb{R}^{40\times 40}$, $i = 60, 61, \ldots, 324$, constructed at each iteration of the algorithm. The matrices M_i are nonsingular. The number of positive and negative eigenvalues are denoted by circles and asterisks, respectively. It appears that the inertia of the matrices M_i varies quite significantly, but the algorithm nevertheless tracks the dominant space very well. Indeed, the angle between the subspace spanned by the eigenvectors corresponding to the 10 largest eigenvalues of A_n and the subspace spanned by the eigenvectors corresponding to the 10 largest eigenvalues of $\tilde{A}_n$ is 6.504e−004.

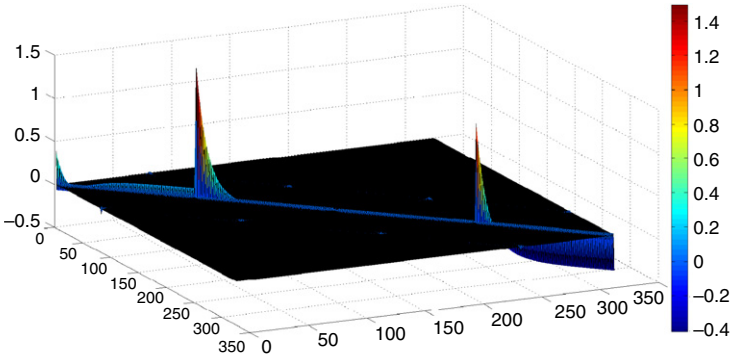

Fig. 10. Plot of the entries of matrix A of Example 4.3.

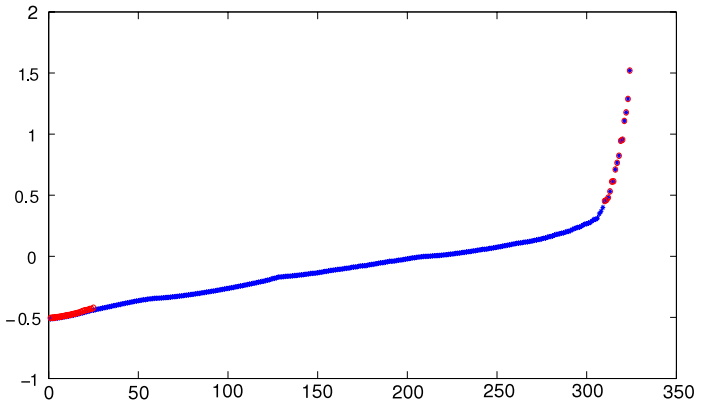

Fig. 11. Plot of the eigenvalues of the matrix A_n (asterisk) and of those of the matrix $\tilde{A}_n$ (circle).

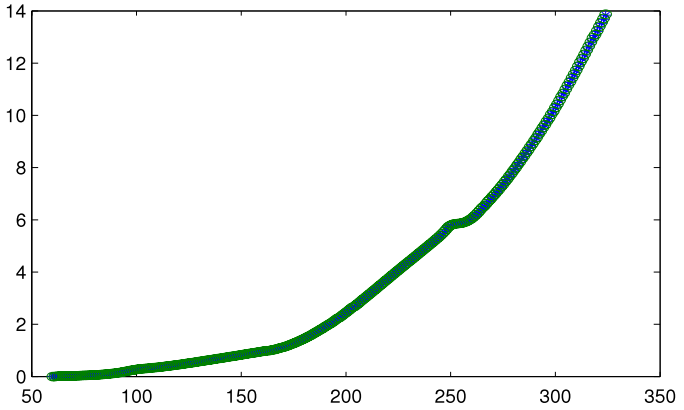

Fig. 12. Plot of $\|A_k - \tilde{A}_k\|_F$ (asterisk) and η_k (circle) of Example 4.1.

5. Conclusions

In this paper, we presented a fast algorithm to compute incrementally the dominant eigenspace of a symmetric indefinite matrix. The overall complexity of the incremental updating technique to compute an $n \times k$ basis matrix U_n for the dominant eigenspace of A_n, is of the order of $6n^2k + O(nk^2)$ and uses only orthogonal updating transformations. The method heavily relies on the anti-triangular form developed in [7], which was shown to be backward stable because of the use of orthogonal transformations. In this paper we analyzed the tracking capabilities of the updating scheme and gave accuracy bounds and computable estimates for these bounds. We also validated those results by a number of convincing examples.

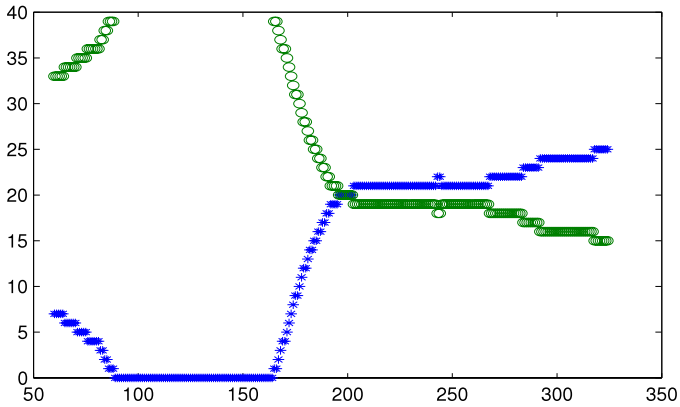

Fig. 13. Plot of the number of positive (circle) and negative (asterisk) eigenvalues of the matrices M_i.

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