The Rotation of Eigenspaces of Perturbed Matrix Pairs

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Abstract

We present new \( \sin \Theta \) theorems for perturbations of positive definite matrix pairs. The rotation of eigenspaces is measured in the matrix dependent scalar product. We assess the sharpness of the new estimates in terms of effectivity quotients (the quotient of the measure of the perturbation and the estimator). Known relative \( \sin \Theta \) theorems for eigenspaces of positive definite Hermitian matrices are included as special cases in our approach. Our experiments indicate that relative \( \sin \Theta \) theorems are asymptotically sharp when the rotation is measured in the appropriate matrix dependent scalar product but not always in the ordinary Euclidean scalar product.

Keywords: matrix pairs, rotation of eigenvectors

1. Introduction and motivation

Given positive definite Hermitian matrix pairs \((H, M)\) and \((\widetilde{H}, \widetilde{M}) = (H + \delta H, M + \delta M)\) and their spectral subspaces \(E\) and \(\widetilde{E}\) of the same dimension we provide estimates on the size of the rotation which moves \(E\) to \(\widetilde{E}\) in the form of the relative \( \sin \Theta \) theorem

\[
\| \sin \Theta_M(E, \widetilde{E}) \| \leq \frac{1}{\text{Gap}_1} \frac{\eta_H}{\sqrt{1 - \eta_H}} + \frac{1}{\text{Gap}_2} \frac{\eta_M}{\sqrt{1 - 2\eta_M}}. 
\]  

In this estimate \( \eta_A = \| A^{-1/2}(A - \widetilde{A})A^{-1/2} \| \) is the usual relative distance between positive definite Hermitian matrices \( A \) and \( \widetilde{A} \), constants \( \text{Gap}_{1,2} \) represent a certain relative distance between the eigenvalues associated with \( E \) and the rest of the spectrum and \( \| \sin \Theta_M(E, \widetilde{E}) \| \) measures the size of the rotation which moves \( E \) to \( \widetilde{E} \) in the scalar product \((x, y)_M = x^* M y\).

For the purpose of comparison, the standard \( \sin \Theta \) theorem for matrix pairs from [17] reads

\[
\| \sin \Theta(E, \widetilde{E}) \| \leq \sqrt{\|H\|^2 + \|M\|^2} \sqrt{\|\delta HP_E\|^2 + \|\delta MP_E\|^2}, 
\]  

where \( P_E \) is the orthogonal projection onto \( E \) and the constants \( \sqrt{\|H\|^2 + \|M\|^2} \) and \( \text{Gap}_3 \) measure the conditioning and certain absolute distance between the eigenvalues associated with \( E \) and the rest of the spectrum, respectively.
We will not discuss in detail the differences between various measures of the spectral gap here. We refer the interested reader to Section 3 for the precise formulation of the measures of the spectral gap which are used in this paper. Here we point out that a relative measure of an eigenvalue gap distinguishes the eigenvalues which are small in magnitude much better than the absolute measure. Further, we point out that the main difference between the relations (1) and (2) lies in the influence of the condition number $\sqrt{\|H\|^2 + \|M\|^2}$. If the matrices $H$ and $M$ originate as discretizations of differential operators, then $\sqrt{\|H\|^2 + \|M\|^2}$ can be so large that bound (2) is useless. On the other hand, estimate (1) will give some useful information in most settings. This can particularly be observed in the case of the matrix pair $(H, I)$. In this case our bound is identical to the standard sin $\Theta$ theorem for a single matrix. This result also holds for unbounded operators in a Hilbert space, see [10]. This indicates that although the norm of the perturbation $\|\delta H\|$ can be infinite, $\eta_H$ can still be finite and bound (1) will give some information on the size of the subspace rotation. For more details on the standard sin $\Theta$ theorems see [5, 10, 14, 15, 17].

We consider the notion of the optimality of subspace rotation estimates in the context of parameter dependent perturbation families. The allowed families of Hermitian perturbations $\delta H_\kappa$ and $\delta M_\kappa$, where $\kappa$ is some indexing parameter, are assumed to satisfy the restrictions

$$
\eta_{H_\kappa} := \|H_\kappa^{-1/2}\delta H_\kappa H_\kappa^{-1/2}\| \\
\lim_{\kappa \to \infty} \eta_{H_\kappa} = 0 \\
\eta_{M_\kappa} := \|M_\kappa^{-1/2}\delta M_\kappa M_\kappa^{-1/2}\| \\
\lim_{\kappa \to \infty} \eta_{M_\kappa} = 0.
$$

By $x^*$ and $H^*$ we denote the transpose or Hermitian transpose of the vector $x$ and the matrix $H$, respectively, as is given by the context. We apply (1) by setting $\tilde{H} = H_\kappa := H + \delta H_\kappa$ and $\tilde{M} = M_\kappa := M + \delta M_\kappa$.

The perturbation families satisfying (3) include perturbations induced by penalty methods for Stokes and Maxwell equations from [18] as well as perturbations introduced while assembling the finite element stiffness matrices by numerical integration as considered in [1]. In [18, Section 4], the authors studied the perturbation of eigenvalues by a very elegant Gerschgorin type argument and in this paper we give an eigenspace counterpart of such a result. For more details see the explicitly solved academic model problem from Appendix A. Note that this family of perturbations is an example of a family of matrix perturbations for which the factor $\sqrt{\|H + \delta H_\kappa\|^2 + \|M + \delta M_\kappa\|^2}$ from (2) explodes even when the norms of the initial matrices $H$ and $M$ are moderate.

Further, note that (3) allows for consideration of the effects of “mass lumping” on the accuracy of the finite element spectral methods. The method of mass lumping amounts to constructing a diagonal matrix $\tilde{M} = M + \delta M$, with $\delta M$ small in some sense. For further information and references, see paper [1] and the academic example from Section 4.1. In Experiment 4.2, we compare our results with those that follow from the standard reference [17]. For the purpose of comparison we use a matrix pair $(H, M)$ which is constructed from the Matrix Market’s CYLSHELL collection. We assume that the perturbation is a random symmetric matrix which is componentwise small.

Let us emphasize that the main contribution of this paper is the new relative sin $\Theta$ theorem for pairs of positive definite matrices. We are not aware of any similar result.
for the rotation of eigenspaces of matrix pairs under the influence of a relatively bounded perturbation of both matrices. Since our result contains the standard sin Θ theorems from [10, 15] as a special case it could be seen as their direct generalization.

Note that estimates of the eigenvector rotation in a matrix dependent scalar product have been used in [12] to analyze the convergence of the Lanczos method. There the authors show how to efficiently compute the estimator in the context of computationally competitive numerical linear algebra procedures. We extend some of those results by giving a new subspace version of some of the estimates, e.g. see appropriate parts of [12, Proposition 3.3 and 3.4] and compare them with our numerical results from Section 4. It is possible that our subspace results could be of technical help when developing a similar analysis of the block Lanczos method.

2. Notations, definitions and a general setting

We consider the following generalized eigenvector problem

\[ Hx = \lambda Mx, \]  

(5)

and the corresponding perturbed one

\[ (H + \delta H)\tilde{x} = \tilde{\lambda}(M + \delta M)\tilde{x}, \]  

(6)

where \( H, M, \tilde{H} \equiv H + \delta H, \tilde{M} \equiv M + \delta M \in \mathbb{C}^{n \times n} \) are Hermitian positive definite matrices.

A pair of positive definite matrices \((H, M)\) can be simultaneously diagonalized. That is, there exists a non-singular matrix \(X\) such that

\[ X^*HX = \Lambda, \quad X^*MX = I, \]  

(7)

where \(\Lambda = \text{diag} (\lambda_1, \ldots, \lambda_n)\), \(\lambda_i \in \mathbb{R}\) for \(i = 1, \ldots, n\). Note that the definition of a positive definite matrix pair is more general, see [17].

Given \(k, 1 \leq k < n\) let us decompose \(X\) as

\[ X = [X_1 \quad X_2], \quad X_1, \in \mathbb{C}^{n \times k} \quad \text{and} \quad X_2 \in \mathbb{C}^{n \times (n-k)}. \]  

(8)

The eigen-decomposition (7) can now be written as

\[ \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} H \begin{bmatrix} X_1 & X_2 \end{bmatrix} = \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix}, \quad \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} M \begin{bmatrix} X_1 & X_2 \end{bmatrix} = \begin{bmatrix} I_k & 0 \\ 0 & I_{n-k} \end{bmatrix}. \]  

(9)

Here we use \(I_m\) to denote the identity matrix in \(\mathbb{C}^m\), \(m \in \mathbb{N}\). From (9) it follows that

\[ HX_1 = MX_1\Lambda_1, \quad HX_2 = MX_2\Lambda_2, \]  

(10)

where \(\Lambda_1 = \text{diag} (\lambda_1, \ldots, \lambda_k) \in \mathbb{C}^{k \times k}\) and \(\Lambda_2 = \text{diag} (\lambda_{k+1}, \ldots, \lambda_n) \in \mathbb{C}^{(n-k) \times (n-k)}\). If \(\min\{|\lambda_i - \lambda_j| : i = 1, \ldots, k, j = k + 1, \ldots, n\} > 0\), then the subspaces \(\text{Ran}(X_1)\) and \(\text{Ran}(X_2)\) are called the spectral subspaces associated with the decomposition (9).
2.1. Measures for perturbations of positive definite matrices

The size of the perturbations $\delta H = \tilde{H} - H$ and $\delta M = M - \tilde{M}$ will be measured relative to the matrices $H, \tilde{H}, M$ and $\tilde{M}$. This means that we express our estimates in terms of the singular values of matrices

$$H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2} \text{ and } M^{-1/2}(M - \tilde{M})\tilde{M}^{-1/2}$$

or

$$H^{-1/2}(H - \tilde{H})H^{-1/2} \text{ and } M^{-1/2}(M - \tilde{M})M^{-1/2}.$$  (12)

Typically, we only use the maximal singular value which corresponds to the spectral norm estimate of these relative perturbations. However, we also consider other unitary invariant matrix norms which can be expressed as functions of all singular values of a matrix.

In this paper, we use $\| \cdot \|_2$, $\| \cdot \|_F$ and $\| \cdot \|$ to denote the spectral matrix norm, the Frobenius norm and any unitary invariant matrix norm, respectively, when there is no danger of confusion.

Lemma 2.1. Let $H$ and $\tilde{H}$ be positive definite matrices and let

$$\eta_H := \|H^{-1/2}(H - \tilde{H})H^{-1/2}\|_2 < 1.$$  

Then for any $x, y \in \mathbb{C}^n$ we have

$$|x^*(H - \tilde{H})x| \leq \eta_H x^*Hx,$$  (13)

$$|x^*(H - \tilde{H})y| \leq \frac{\eta_H}{\sqrt{1 - \eta_H}} \sqrt{x^*Hx \cdot x^*Hx},$$  (14)

$$\|H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2}\| \leq \frac{1}{\sqrt{1 - \eta_H}} \|H^{-1/2}(H - \tilde{H})H^{-1/2}\|.$$  (15)

Proof. The proof is by direct computation, see also [10]. □

2.2. Relations between subspaces in the matrix dependent scalar product

We will now compare two $m$ dimensional subspaces of $\mathbb{C}^n$ in the scalar product $(x, y)_M = x^*M y$, $x, y \in \mathbb{C}^n$ which is dependent on a positive definite Hermitian matrix $M \in \mathbb{C}^{n \times n}$. We will first present the theory in the Euclidean scalar product and then switch to $(\cdot, \cdot)_M$. Let $X, Y \in \mathbb{C}^{n \times m}$ be such that $X^*X = Y^*Y = I_m$. Then $P_{\text{Ran}(X)} = XX^*$ and $P_{\text{Ran}(Y)} = YY^*$ are orthogonal projections onto the column spaces of $X$ and $Y$. We denote these column spaces by $\text{Ran}(X)$ and $\text{Ran}(Y)$ and compare them analytically by analyzing the spectral properties of the product $(I - P_{\text{Ran}(X)})P_{\text{Ran}(Y)}$. Counted according to their multiplicity, the $m$ largest singular values of $(I - P_{\text{Ran}(X)})P_{\text{Ran}(Y)}$ are called the sines of the angle between the

1According to von Neumann’s theory, unitary invariant matrix norms can be expressed as symmetric gauge functions of the singular values of a matrix, see [17].
subspaces \( \text{Ran}(X) \) and \( \text{Ran}(Y) \). In matrix notation, they are exactly the \( m \) singular values of the matrix

\[
S(X, Y) = (I - XX^*)Y.
\]

Let \( \| \cdot \| \) be a unitary invariant matrix norm, then \( \|S(X, Y)\| \) is a measure of the size of the “smallest” rotation\(^2\) in \( \mathbb{C}^n \) which would move the subspace \( \text{Ran}(X) \) onto \( \text{Ran}(Y) \). For more discussion on the optimality properties of the rotations — represented by unitary matrices — which move \( \text{Ran}(X) \) onto \( \text{Ran}(Y) \) and their relationship to singular values of \( S(X, Y) \) see [5, Section 4.].

In this paper we analyze the angles between subspaces \( \text{Ran}(X) \) and \( \text{Ran}(Y) \) in the scalar product \((\cdot, \cdot)_M\). To this end, let \( X^*MX = Y^*MY = I_m \). The sines of the angle between \( \text{Ran}(X) \) and \( \text{Ran}(Y) \) in the \( M \)-scalar product are now the \( m \)-singular values of the matrix

\[
S^M(X, Y) = M^{1/2}(I - XX^*M)Y.
\]

For more details on angles between subspaces of \( \mathbb{C}^n \), see [5, 13]. We point out the following important observation from [13, Theorem 4.2]. The sines of the angle between the spaces \( \text{Ran}(X) \) and \( \text{Ran}(Y) \) in the \( M \) dependent scalar product are the same as the sines of the angle between the spaces \( \text{Ran}(M^{1/2}X) \) and \( \text{Ran}(M^{1/2}Y) \) in the Euclidean scalar product.

Subsequently, we also have a similar alternative characterization of the sines of the angle between the subspaces. Let \( X = [X_1 \hspace{1em} X_2], X_1 \in \mathbb{C}^{n \times k}, X_2 \in \mathbb{C}^{n \times (n-k)} \) and let \( Y = [Y_1 \hspace{1em} Y_2], Y_1 \in \mathbb{C}^{n \times k}, Y_2 \in \mathbb{C}^{n \times (n-k)} \) be nonsingular matrices such that \( X^*MX = Y^*MY = I \). Then singular values of the matrix

\[
\sin \Theta_M(X_1, Y_1) = Y_2^*M X_1
\]

and the matrix \( S^M(X_1, Y_1) \) coincide. By \( \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(Y_1)) \) we denote the diagonal matrix with singular values — ordered in the descending order — of the matrix \( \sin \Theta_M(X_1, Y_1) \) on its diagonal. Obviously, the matrix \( \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(Y_1)) \) depends solely on the subspaces \( \text{Ran}(X_1) \) and \( \text{Ran}(Y_1) \) and not on the matrices \( X_1 \) and \( Y_1 \).

The following relationship between the matrices which are orthogonal in the \( M \)-dependent and \( \tilde{M} \)-dependent (\( \tilde{M} = M + \delta M \)) scalar products is important for our perturbation problem. For \( \tilde{X} \in \mathbb{C}^n \) such that \( \tilde{X}^*\tilde{M}\tilde{X} = I \), we compute

\[
\tilde{X}^*M\tilde{X} = \tilde{X}^*\tilde{M}\tilde{X} - \tilde{X}^*\delta M\tilde{X} = I - \tilde{X}^*\delta M\tilde{X}.
\]

This identity implies that the matrix \( I - \tilde{X}^*\delta M\tilde{X} \) is positive definite and so it has the block Cholesky decomposition \( GG^* = I - \tilde{X}^*\delta M\tilde{X} \), where

\[
G = \begin{bmatrix} G_{11} & 0 \\ G_{21} & G_{22} \end{bmatrix},
\]

\(^2\)Such rotation exists and is unique if all of the sines of the angle between \( \text{Ran}(X) \) and \( \text{Ran}(Y) \) are strictly smaller than one.
and $G_{11} \in \mathbb{C}^{k \times k}$, $G_{21} \in \mathbb{C}^{(n-k) \times k}$, $G_{22} \in \mathbb{C}^{(n-k) \times (n-k)}$. Direct computation proves that the columns of $XG^{-*}$ are $M$-orthogonal. Similarly, we conclude that the columns of $X_1G_{11}^{-*}$, $G_{11}G_{11}^{-*} = I_m - \tilde{X}_1^T \delta M \tilde{X}_1$ are also $M$-orthogonal.

Let $\tilde{X} = [\tilde{X}_1 \ \tilde{X}_2]$ be an auxiliary $M$-orthogonal matrix, that is let $\tilde{X}^*M\tilde{X} = I$, then for such $\tilde{X}_1$ and $\tilde{X}_1G_{11}^{-*}$ the following holds

$$\| \sin \Theta_M(\text{Ran}(\tilde{X}_1), \text{Ran}(\tilde{X}_1)) \| = \| \tilde{X}_2^*M\tilde{X}_1G_{11}^{-*} \|,$$

(17)

for any unitary invariant norm $\| \cdot \|$.

With this observation we formulate the main lemma which will describe the geometrical setting of our perturbation analysis.

**Lemma 2.2.** Let $M$ and $\tilde{M} = M + \delta M$ be positive definite matrices and let $X$, $\tilde{X}$ and $\tilde{X}$ be such that $X^*MX = \tilde{X}^*\tilde{M}\tilde{X} = \tilde{X}^*\tilde{M}\tilde{X} = I$. If $X$, $\tilde{X}$ and $\tilde{X}$ are decomposed as in (8), then

$$\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \leq \| \tilde{X}_2^*M\tilde{X}_1 \| + \| \tilde{X}_2^*M\tilde{X}_1G_{11}^{-*} \|.$$

(18)

**Proof.** Let $X^*Y = Y^*Y = I_m$, then using [17, Theorem II 4.10.] one can write

$$\| \sin \Theta(\text{Ran}(X), \text{Ran}(Y)) \| = \| XX^* - YY^* \|,$$

(19)

for any unitary invariant norm $\| \cdot \|$. Note that the columns of matrices $X_1^M = M^{1/2}X_1$, $\tilde{X}_1^M = M^{1/2}\tilde{X}_1$ and $\tilde{X}_1G_{11}^{-*} = M^{1/2}\tilde{X}_1G_{11}^{-*}$ are unitary, thus using (19) we obtain

$$\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| = \| P_{X_1} - P_{\tilde{X}_1} \| = \| \tilde{X}_2^*M\tilde{X}_1 \|,$$

(20)

where $P_{X_1} = X_1^M(X_1^M)^*$ and $P_{\tilde{X}_1} = \tilde{X}_1^M(\tilde{X}_1^M)^*$. Similarly,

$$\| \sin \Theta_M(\text{Ran}(\tilde{X}_1), \text{Ran}(\tilde{X}_1)) \| = \| P_{\tilde{X}_1} - P_{\tilde{X}_1} \| = \| \tilde{X}_2^*M\tilde{X}_1G_{11}^{-*} \|,$$

where $P_{\tilde{X}_1} = \tilde{X}_1^M(\tilde{X}_1^M)^*$ and $P_{\tilde{X}_1} = \tilde{X}_1^M(\tilde{X}_1^M)^*$. The proof of the lemma now follows by the application of the triangle inequality for the unitary invariant norm $\| \cdot \|$. □

**3. The main result**

In the pioneering analysis from [2, Lemma 2 in Section 4], the problem of the change of the eigenvalues of a pair of positive definite matrices has been completely solved. Given positive definite matrix pairs $(H_1, M_1)$ and $(H_2, M_2)$ and their eigenvalues $\lambda_1^{(1)} \leq \cdots \leq \lambda_n^{(1)}$ and $\lambda_1^{(2)} \leq \cdots \leq \lambda_n^{(2)}$, counted according to their multiplicity, we have the estimate

$$\frac{1 - \| H_2^{-1/2}(H_1 - H_2)H_2^{-1/2} \|_2}{1 + \| M_2^{-1/2}(M_1 - M_2)M_2^{-1/2} \|_2} \leq \frac{\lambda_1^{(1)}}{\lambda_1^{(2)}} \leq \frac{1 + \| H_2^{-1/2}(H_1 - H_2)H_2^{-1/2} \|_2}{1 - \| M_2^{-1/2}(M_1 - M_2)M_2^{-1/2} \|_2},$$

(21)

for every $i = 1, \cdots, n$. Here we tacitly assume that all of the quotients are finite.
This result has been proved by analyzing the eigenvalue change in the transformations \((H_1, M_1) \mapsto (H_2, M_1)\) and then \((H_2, M_1) \mapsto (H_2, M_2)\). The two partial results were then joined together to obtain (21), cf. [2, Section 4]. We note that there is no known eigensubspace counterpart of this result, so far.

We now repeat this procedure for the eigenvector case and thus obtain an eigensubspace companion of this result. The main tools in our analysis are sharp estimates for the solution of the structured Sylvester equations from [15, Lemma 2.4] and [15, Lemma 2.3]. That is, we consider the structured Sylvester equations\(^3\)

\[
AX - XB = A^{1/2}CB^{1/2} \\
AX - XB = CB. \tag{23}
\]

Finally, we use identity (18) to join the two partial results into the main theorem.

3.1. Comparison of \((H, M)\) and \((\tilde{H}, M)\)

Now we will state our first theorem. The matrices \(H, M\) and \(\tilde{H} = H + \delta H\) are assumed to be positive definite and so decomposition (9) reads

\[
X^*HX = \Lambda, \quad X^*MX = I, \quad \tilde{X}^*\tilde{H}\tilde{X} = \tilde{\Lambda}, \quad \tilde{X}^*M\tilde{X} = I, \tag{24}
\]

where \(\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)\), \(\tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)\), \(\lambda_i, \tilde{\lambda}_i \in \mathbb{R}\), for \(i = 1, \ldots, n\). We will also use the notation and the conclusions of Lemma 2.1 without further comments.

**Theorem 3.1.** Let \(X = [X_1 \quad X_2]\) and \(\tilde{X} = \begin{bmatrix} \tilde{X}_1 & \tilde{X}_2 \end{bmatrix}\) be non-singular matrices from (24) which are assumed to be partitioned as in (8) and let \(\min_{i=k+1, \ldots, n} |\lambda_i - \tilde{\lambda}_j|/(\lambda_i\tilde{\lambda}_j)^{-1/2} > 0\). Then

\[
\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \leq \frac{\|H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2}\|}{\min_{i=k+1, \ldots, n} |\lambda_i - \tilde{\lambda}_j|/(\lambda_i\tilde{\lambda}_j)^{1/2}}. \tag{25}
\]

**Proof.** The identity \(X^*HX = \Lambda\) implies the relationship

\[
H^{1/2}X = U\Lambda^{1/2}, \tag{26}
\]

where \(U = [U_1 \quad U_2] = H^{1/2}X\Lambda^{-1/2}\) is unitary and has the block structure conforming to the structure of \(X\). A similar identity also holds for perturbed quantities.

Let now \(\Lambda_2 = \text{diag}(\lambda_{k+1}, \ldots, \lambda_n)\), and \(\tilde{\Lambda}_1 = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_k)\) be the diagonal matrices such that \(HX_2 = MX_2\Lambda_2, \tilde{H}\tilde{X}_1 = M\tilde{X}_1\tilde{\Lambda}_1\). We expand the identity \(\tilde{H}\tilde{X}_1 = (H + \delta H)\tilde{X}_1 = M\tilde{X}_1\tilde{\Lambda}_1\) and multiply it by \(X_2^*\) from the left to obtain

\[
X_2^*H\tilde{X}_1 - X_2^*M\tilde{X}_1\tilde{\Lambda}_1 = -X_2^*\delta H\tilde{X}_1.
\]

---

\(^3\)The solution of (22) is presented in [15, Lemma 2.4]. This equation has also been analyzed in the infinite dimensional setting in [10]. Equation (23) has been analyzed in [15, Lemma 2.3], see also [14].
Using the fact that $HX_2 = MX_2\Lambda_2$, this identity can be transformed into
\[ \Lambda_2X^*_2M\tilde{X}_1 - X^*_2M\tilde{X}_1\Lambda_1 = -X^*_2\delta H\tilde{X}_1. \] (27)
We rewrite the right-hand side of (27) as
\[ X^*_2\delta H\tilde{X}_1 = X^*_2H^{1/2}H^{-1/2}\delta H\tilde{H}^{-1/2}\tilde{H}^{1/2}\tilde{X}_1, \] (28)
which together with (26) gives
\[ X^*_2\delta H\tilde{X}_1 = \Lambda_2^{1/2}U^*_2H^{-1/2}\delta H\tilde{H}^{-1/2}\tilde{U}_1\Lambda_1^{1/2}. \]
The above equality and (27) now yield
\[ \Lambda_2X^*_2M\tilde{X}_1 - X^*_2M\tilde{X}_1\Lambda_1 = -\Lambda_2^{1/2}U^*_2H^{-1/2}\delta H\tilde{H}^{-1/2}\tilde{U}_1\Lambda_1^{1/2}. \] (29)
This identity can be recognized as the structured Sylvester equation from (22).
We apply [15, Lemma 2.4] on (29) to obtain the bounds on the solution of the structured Sylvester equation for any unitary invariant norm $\| \cdot \|$ (see also [14]). This computation yields an estimate of $\| \sin \Theta_M(\tilde{X}_1, X_1) \|$. We note that $\| \sin \Theta_M(\tilde{X}_1, X_1) \| = \| \sin \Theta_M(X_1, \tilde{X}_1) \|$ and so we conclude the proof of the theorem. ■

3.2. Comparison of $(\tilde{H}, M)$ and $(\tilde{H}, \tilde{M})$

Now let the matrices $\tilde{X}$ and $\tilde{X}$ be given such that
\[ \tilde{X}^*\tilde{H}\tilde{X} = \tilde{\Lambda}, \quad \tilde{X}^*M\tilde{X} = I, \quad \tilde{X}^*\tilde{H}\tilde{X} = \tilde{\Lambda}, \quad \tilde{X}^*M\tilde{X} = I, \] (30)
where $\tilde{\Lambda} = \text{diag}(\hat{\lambda}_1, \ldots, \hat{\lambda}_n)$, and $\tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_n)$, and $\hat{\lambda}_i, \tilde{\lambda}_i \in \mathbb{R}$, for $i = 1, \ldots, n$. We also assume that $\tilde{X} = \begin{bmatrix} \tilde{X}_1 & \tilde{X}_2 \end{bmatrix}$ and $\tilde{X} = \begin{bmatrix} \tilde{X}_1 & \tilde{X}_2 \end{bmatrix}$ is the block matrix representation conforming to (9).

\[ \begin{array}{ccc}
\tilde{\lambda}_1 & \tilde{\lambda}_2 \\
0 & \alpha & \alpha + \delta
\end{array} \]

Figure 1: Spectral configuration for Theorem 3.2 as given by condition (32).

The following theorem contains the upper bound for $\| \tilde{X}^*_2M\tilde{X}_1 \|$. Here $\| \cdot \|$ stands for any unitary invariant norm and $\| \cdot \|_2$ denotes the spectral norm.

**Theorem 3.2.** Let $\tilde{H}\tilde{X}_2 = M\tilde{X}_2\tilde{\Lambda}_2$, $\tilde{H}\tilde{X}_1 = \tilde{M}\tilde{X}_1\tilde{\Lambda}_1$, where $\tilde{\Lambda}_2 = \text{diag}(\hat{\lambda}_{k+1}, \ldots, \hat{\lambda}_n)$, and $\tilde{\Lambda}_1 = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_k)$ are the conforming diagonal matrices as in (9). If
\[ \| \tilde{\Lambda}_2 \|_2 \leq \alpha \quad \text{and} \quad \| \tilde{\Lambda}_2^{-1} \|_2^{-1} \geq \alpha + \delta \quad \text{or} \] (31)
\[ \| \tilde{\Lambda}_2^{-1} \|_2^{-1} \geq \alpha + \delta \quad \text{and} \quad \| \tilde{\Lambda}_1 \|_2 \leq \alpha \] (32)
\[ \| \tilde{X}_2^* M \tilde{X}_1 \| \leq \frac{\| M^{-1/2}(M - \tilde{M})\tilde{M}^{-1/2} \|}{\alpha + \delta}. \]  

(33)

Proof. We start by multiplying the identity \( \tilde{H} \tilde{X}_1 = \tilde{M} \tilde{X}_1 \tilde{\Lambda}_1 \) by \( \tilde{X}_2^* \) from the left to obtain
\[ \tilde{X}_2^* \tilde{H} \tilde{X}_1 - \tilde{X}_2^* (M - \delta M) \tilde{X}_1 \tilde{\Lambda}_1 = 0. \]

The identity \( \tilde{H} \tilde{X}_2 = M \tilde{X}_2 \tilde{\Lambda}_2 \) now implies
\[ \tilde{\Lambda}_2 \tilde{X}_2^* M \tilde{X}_1 - \tilde{X}_2^* M \tilde{X}_1 \tilde{\Lambda}_1 = -\tilde{X}_2^* \delta M \tilde{X}_1 \tilde{\Lambda}_1. \]  

(34)

The right-hand side of (34) can be rewritten as
\[ \tilde{X}_2^* \delta M \tilde{X}_1 = \tilde{Q}_2^* M^{1/2} M^{-1/2} \tilde{M}^{-1/2} \tilde{M}^{-1/2} \tilde{\Lambda}_1. \]  

(35)

On the other hand, identity (30) implies that the matrices \( \tilde{Q}_2 \equiv \tilde{X}_2^* M^{1/2} \) and \( \tilde{Q}_1 \equiv \tilde{M}^{1/2} \tilde{X}_1 \) have unitary columns, which together with (35) gives
\[ \tilde{X}_2^* \delta M \tilde{X}_1 = \tilde{Q}_2^* M^{-1/2} \tilde{M}^{-1/2} \tilde{M}^{-1/2} \tilde{\Lambda}_1. \]

We now apply [15, Lemma 2.3] to obtain a bound on the solution of a structured Sylvester equation (34) in any unitary invariant norm, cf. [14].

Conditions (31) and (32) imply that the spectra of \( \tilde{\Lambda}_2 \) and \( \tilde{\Lambda}_1 \) are in a mutually dominant/subordinate position. This arrangement of the spectra will enable us to prove more refined estimates for the rotation of the associated spectral subspaces. Therefore we will — for easier reference — give this condition a name.

**Definition 3.3 (Condition-DS).** We say that square Hermitian matrices \( A \) and \( B \) satisfy the Condition-DS if there exist numbers \( \alpha > 0 \) and \( \delta > 0 \) such that
\[ \| B \|_2 \leq \alpha \quad \text{and} \quad \| A^{-1} \|_2^1 \geq \alpha + \delta \]  

(36)

\[ \| B^{-1} \|_2^{-1} \geq \alpha + \delta \quad \text{and} \quad \| A \|_2 \leq \alpha \]  

(37)

holds.

**Remark 3.4.** Let matrices \( \tilde{\Lambda}_2 \) and \( \tilde{\Lambda}_1 \) satisfy the Condition-DS then for all \( p, 1 \leq p \leq \infty \) we have the estimate
\[ \frac{\delta}{\alpha + \delta} \geq \min_{i=k+1, \ldots, n} \frac{|\tilde{\lambda}_i - \tilde{\lambda}_j|}{\left(\lambda_i^p + \lambda_j^p\right)^{1/p}}. \]  

(38)

The result also holds for square matrices \( \tilde{\Lambda}_2 \) and \( \tilde{\Lambda}_1 \) which are not diagonal.
3.3. The main result

As indicated in Lemma 2.2, we can obtain a bound for

$$\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \|$$

as the sum of the bounds for

$$\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| = \| \tilde{X}_1^* M X_1 \|,$$

and

$$\| \sin \Theta_M(\text{Ran}(\tilde{X}_1), \text{Ran}(\tilde{X}_1)) \| = \| \tilde{X}_1^* M \tilde{X}_1 G_{11}^* \|.$$ 

This is our main theorem.

**Theorem 3.5.** Let \((H, M), (\tilde{H}, M)\) and \((\tilde{H}, \tilde{M})\) be pairs of positive definite Hermitian matrices. Let \(X = [X_1 \; X_2], \tilde{X} = [\tilde{X}_1 \; \tilde{X}_2]\) and \(\tilde{X} = [\tilde{X}_1 \; \tilde{X}_2]\) be non-singular matrices which simultaneously diagonalize these matrix pairs respectively, as in Theorem 3.1 and 3.2. If

$$\eta_M = \| M^{-1/2} \delta M M^{-1/2} \|_2 < \frac{1}{2},$$

then

$$\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \leq \frac{\| H^{-1/2} \delta H \tilde{H}^{-1/2} \|}{\min_{i=k+1, \ldots, n} \frac{|\lambda_i - \lambda_j|}{(\lambda_i \lambda_j)^{1/2}}} + \frac{\sqrt{1 - \eta_M}}{\sqrt{1 - 2 \eta_M}} \frac{\| M^{-1/2} \delta M \tilde{M}^{-1/2} \|}{\min_{i=k+1, \ldots, k} \frac{|\tilde{\lambda}_i - \tilde{\lambda}_j|}{(\hat{\lambda}_p^i + \hat{\lambda}_p^j)^{1/p}}}$$

for any \(p, 1 \leq p \leq \infty\). Here we use \(\lambda_i, \hat{\lambda}_i\) and \(\tilde{\lambda}_i, i = 1, \ldots, n\) to denote the eigenvalues of \((H, M), (\tilde{H}, M)\) and \((\tilde{H}, \tilde{M})\) respectively. We assume the ordering of eigenvalues as in (9) and we use \(\delta M = M - \tilde{M}\) and \(\delta H = H - \tilde{H}\).

**Proof.** Using Theorems 3.1 and 3.2, Lemma 2.2, relation (38) and the multiplicative properties of unitary invariant matrix norms, one gets

$$\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \leq \frac{\| H^{-1/2} \delta H \tilde{H}^{-1/2} \|}{\min_{i=k+1, \ldots, n} \frac{|\lambda_i - \lambda_j|}{(\lambda_i \lambda_j)^{1/2}}} + \frac{\| M^{-1/2} \delta M \tilde{M}^{-1/2} \|}{\min_{i=k+1, \ldots, k} \frac{|\tilde{\lambda}_i - \tilde{\lambda}_j|}{(\hat{\lambda}_p^i + \hat{\lambda}_p^j)^{1/p}}} \| G_{11}^{-1} \|_2,$$

where \(G_{11} = \sqrt{I - \tilde{X}_1^* \delta M \tilde{X}_1} \).
In the rest of the proof we compute a bound of \( \|G_{11}^{-1}\|_2 \) in terms of \( \eta_M \). Using the \( \widetilde{M} \)-orthogonality of \( \widetilde{X} \), it can be easily seen that \( \widetilde{X} \) and \( M^{-1/2}(I + M^{-1/2}\delta MM^{-1/2})^{-1/2} \) are unitarily similar, that is, there exists a unitary matrix \( Q \) such that
\[ \widetilde{X} = M^{-1/2}(I + M^{-1/2}\delta MM^{-1/2})^{-1/2}Q. \]
The inequality
\[ \| (I - \widetilde{X}_1^*\delta M\widetilde{X}_1)^{-1/2} \|_2 \leq \frac{1}{\sqrt{1 - \|\widetilde{X}_1^*\delta M\widetilde{X}_1\|_2}} \leq \frac{1}{\sqrt{1 - \|\widetilde{X}_1^*\delta M\widetilde{X}_1\|_2}} \]
follows by the spectral calculus. Set \( W = M^{-1/2}\delta MM^{-1/2} \), then (41) implies
\[ \|\widetilde{X}_1^*\delta M\widetilde{X}_1\|_2 = \|(I + W)^{-1/2}W(I + W)^{-1/2}\|_2 \leq \frac{\eta_M}{1 - \eta_M}. \]
Finally, by inserting (43) in (42) one gets
\[ \| (I - \widetilde{X}_1^*\delta M\widetilde{X}_1)^{-1/2} \|_2 \leq \frac{\sqrt{1 - \eta_M}}{\sqrt{1 - 2\eta_M}}. \]
Combining (44) with (40) we obtain the statement of the theorem. ■

An alternative version can be obtained using Lemma 2.1.

**Corollary 3.6.** Under the assumptions of Theorem 3.5 we have the estimate
\[ \| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\widetilde{X}_1)) \| \leq \frac{\|H^{-1/2}\delta HH^{-1/2}\|}{\text{RelGap} \sqrt{1 - \eta_H}} + \frac{\|M^{-1/2}\delta MM^{-1/2}\|}{\text{RelGap}_p \sqrt{1 - 2\eta_M}}, \]
where
\[ \text{RelGap} = \min_{i=1,\ldots,k} \frac{|\lambda_i - \lambda_j|}{(\lambda_i\lambda_j)^{1/2}}, \quad \text{RelGap}_p = \min_{i=1,\ldots,k} \frac{|\tilde{\lambda}_i - \tilde{\lambda}_j|}{(\tilde{\lambda}_i^p + \tilde{\lambda}_j^p)^{1/p}}. \]

### 3.4. A gap in the spectrum and spectral dichotomy

The theorems of the preceding sections are given in terms of the eigenvalues \( \lambda_i, \tilde{\lambda}_i \) and \( \hat{\lambda}_i \), \( i = 1, \ldots, n \) of matrix pairs \( (H, M) \), \( (\tilde{H}, M) \) and \( (\hat{H}, M) \). In a certain sense, the matrix pair \( (\tilde{H}, M) \) is auxiliary in our perturbation formulation. Subsequently, its eigenvalues should not appear in the estimates as they do in Theorem 3.5.

This deficiency can be removed by the use of (21). The situation is best illustrated in the case in which matrices \( \Lambda_2 \) and \( \hat{\Lambda}_1 \) satisfy the Condition-DS and \( \eta_H \) and \( \eta_M \) are smaller then \( \frac{\delta}{3(\delta + \alpha)} \). Then, by (21) one directly computes that matrices \( \hat{\Lambda}_2 \) and \( \hat{\Lambda}_1 \) satisfy the Condition-DS with the same \( \alpha > 0 \) and \( \delta > 0 \). We do not explicitly present this technical result, cf. reference [11] for further technical details from the relative perturbation theory. We rather present a corollary which can be obtained for general \( \alpha \) and \( \alpha + \delta \) — regardless of the formula by which they are computed — in the situation when both matrix pairs \( \Lambda_2 \) and \( \hat{\Lambda}_1 \) as well as \( \hat{\Lambda}_2 \) and \( \hat{\Lambda}_1 \) satisfy the Condition-DS with same constants \( \alpha > 0 \) and \( \delta > 0 \).
Thus we continue the proof from there; that is, one can write:

\[
\| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \leq \frac{1}{\sqrt{\alpha(\alpha + \delta)}} \cdot \left\| H^{-1/2} \delta HH^{-1/2} \right\| \sqrt{1 - \eta_H} + \frac{1}{\delta + \alpha} \cdot \left\| M^{-1/2} \delta MM^{-1/2} \right\| \sqrt{1 - 2\eta_M}.
\]

(47)

3.4.1. A result for the Frobenius norm

Theorem 3.2 requires special arrangement of the spectra — which we call the Condition-DS — of \( \hat{\Lambda}_1 \) and \( \hat{\Lambda}_2 \). The reason for this lies in the analysis of the structured Sylvester equation (23); see the comment in the introduction to [14].

This limitation can be removed by using the Frobenius norm instead of the spectral norm. Our next theorem contains a perturbation bound similar to the one from Theorem 3.2 given for \( \| \hat{X}_2^* M \tilde{X}_1 \|_F \), without any additional assumptions on the spectral configuration of the pair \((H, M)\). To state the theorem, we need a new measure of the relative gap in the spectrum. We set

\[
\text{RelGap}_{\text{comp}} := \min_{i=k+1, \ldots, n} \frac{|\hat{\lambda}_i - \tilde{\lambda}_j|}{\tilde{\lambda}_j}.
\]

(48)

Theorem 3.8. Let \((\tilde{H}, M), (\hat{H}, \hat{M})\), \( \hat{X} = [\hat{X}_1 \hat{X}_2] \) and \( \tilde{X} = [\tilde{X}_1 \tilde{X}_2] \), be as in Theorem 3.2 and let \( \text{RelGap}_{\text{comp}} > 0 \). Then

\[
\| \hat{X}_2^* M \tilde{X}_1 \|_F \leq \min_{i=k+1, \ldots, n} \frac{|\hat{\lambda}_i - \tilde{\lambda}_j|}{\tilde{\lambda}_j} = \frac{\| M^{-1/2} \delta MM^{-1/2} \|_F}{\text{RelGap}_{\text{comp}}},
\]

(49)

Here we use \( \hat{\lambda}_i \) and \( \tilde{\lambda}_i \), \( i = 1, \ldots, n \) to denote the eigenvalues of \((\tilde{H}, M)\) and \((\hat{H}, \hat{M})\) respectively. We assume the ordering of eigenvalues as in (9).

Proof. The first part of the proof is similar to the proof of Theorem 3.2 up to equality (35). Thus we continue the proof from there; that is, one can write:

\[
\hat{\Lambda}_2 \hat{X}_2^* M \tilde{X}_1 - \hat{X}_2^* M \tilde{X}_1 \hat{\Lambda}_1 = -\hat{X}_2^* \delta M \tilde{X}_1 \tilde{\Lambda}_1,
\]

(50)

and

\[
\hat{X}_2^* \delta M \tilde{X}_1 = \hat{Q}_2^* M^{-1/2} \delta M \tilde{M}^{-1/2} \hat{Q}_1,
\]

(51)

where \( \hat{Q}_2 \equiv \hat{X}_2^* M^{1/2} \) and \( \hat{Q}_1 \equiv \hat{M}^{1/2} \hat{X}_1 \) have unitary columns.

By interpreting (50) and (51) componentwise, it follows

\[
(\hat{\Lambda}_2)_{ij}(\hat{X}_2^* M \tilde{X}_1)_{ij} - (\hat{X}_2^* M \tilde{X}_1)_{ij}(\tilde{\Lambda}_1)_{jj} = -(\hat{Q}_2^* M^{-1/2} \delta M \tilde{M}^{-1/2} \hat{Q}_1)_{ij}(\tilde{\Lambda}_1)_{jj},
\]

12
or
\[
(\hat{X}_2^* M \tilde{X}_1)_{ij} = -\frac{(\hat{\Lambda}_1)_{jj}}{(\hat{\Lambda}_2)_{ii} - (\hat{\Lambda}_1)_{jj}} \left( (\hat{Q}_2)_{(i,j)}^* M^{-1/2} \delta M \tilde{M}^{-1/2} (\tilde{Q}_1)_{(i,j)} \right),
\]  \tag{52}

where \((Q)_{(i,j)}\) denotes the \(j\)-th column of the matrix \(Q\).

By computing the Frobenius norm from (52) we have
\[
\|\hat{X}_2^* M \tilde{X}_1\|_F^2 = \sum_{i=k+1}^{n} \sum_{j=1}^{k} \frac{1}{(\hat{\Lambda}_2)_{ii} - (\hat{\Lambda}_1)_{jj}}^2 \left( (\hat{Q}_2)_{(i,j)}^* M^{-1/2} \delta M \tilde{M}^{-1/2} (\tilde{Q}_1)_{(i,j)} \right)^2, \tag{53}
\]

which gives
\[
\|\hat{X}_2^* M \tilde{X}_1\|_F \leq \frac{\|\hat{Q}_2^* M^{-1/2} \delta M \tilde{M}^{-1/2} \tilde{Q}_1\|_F}{\text{RelGap}_{\text{comp}}}. \tag{54}
\]

The statement of the theorem follows from the unitary invariance of the Frobenius norm. \(\blacksquare\)

We can now give a Frobenius norm version of Theorem 3.5.

**Theorem 3.9.** Let \((H, M)\) be a Hermitian pair and let \((\tilde{H}, \tilde{M})\) be the perturbed pair. Let \(X = [X_1 \ X_2]\) and \(\tilde{X} = [\tilde{X}_1 \ \tilde{X}_2]\) be non-singular matrices which simultaneously diagonalize the pairs \((H, M)\) and \((\tilde{H}, \tilde{M})\). If the spectra are separated so that \(\text{RelGap}_{\text{comp}} > 0\) and \(\text{RelGap} > 0\), where \(\text{RelGap}\) is defined in Corollary 3.6, then
\[
\|\sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1))\|_F \leq \frac{\|H^{-1/2} \delta H \tilde{H}^{-1/2}\|_F}{\text{RelGap}} + \frac{\|M^{-1/2} \delta M \tilde{M}^{-1/2}\|_F}{\text{RelGap}_{\text{comp}}}. \tag{55}
\]

We assume the ordering of eigenvalues as in (9).

4. Numerical examples

In this section we will experimentally consider a family of parameter dependent model problems. The estimate of the type \(\text{Left}(\kappa) \leq \text{Right}(\kappa)\), where \(\kappa \in \mathbb{R}\) is a parameter, is considered asymptotically sharp if
\[
\lim_{\kappa \to \infty} \frac{\text{Left}(\kappa)}{\text{Right}(\kappa)} = 1. \tag{56}
\]

Such property of an estimator is sometimes called (e.g. in the finite element literature) the asymptotic exactness. Also, the quotient \(\frac{\text{Left}(\kappa)}{\text{Right}(\kappa)}\) is called the effectivity quotient. In Appendix A we will construct an explicit example of a matrix where our estimates are asymptotically sharp. The purpose of this section is to experimentally compare the effectivity quotients of several \(\sin \Theta\) theorems.
4.1. A Matrix Market example

We choose the test matrix $H$ from the set CYLSHELL from [16] as our first example. From this test set we take the matrix sirmq4m1.mtx which is a real symmetric positive definite $5489 \times 5489$ matrix with 143300 entries. This matrix is obtained by finite element discretization of an octant of a cylindrical shell. The ends of the cylinder are free.

We will perform two experiments with this matrix to simulate the effects which are induced by

1) random componentwise perturbations,

2) parameter dependent perturbations.

4.1.1. Random componentwise perturbations of a pair $(H, M)$

We will consider the generalized eigenvalue problem

$$Hx = \lambda Mx,$$

where the matrix $H$ is taken from the Matrix Market basis, see [16]. For the matrix $M$ we take a diagonal matrix $\text{diag}(1:n)$ and we consider random perturbations $\delta H$ and $\delta M$, which satisfy

$$|((\delta H)_{ij}| \leq \eta |H_{ij}|, \quad |((\delta M)_{ij}| \leq \eta |M_{ij}|,$$

where $\eta = 10^{-8}$ — the single precision roundoff constant. We point out that these assumptions allow that both the norm of the matrix $M$ as well as the norm of the perturbation $\delta M$ could explode as $n \to \infty$. This is a reasonable choice for our method, since the technique of our proof can readily be adapted to yield the same result for some unbounded pair of operators in a Hilbert space. The experiment is designed to illustrate that our bound is fine enough to detect an effect of a perturbation this small.

As a comparison, we consider one of the best known standard perturbation bounds for matrix pairs as given by the theorem of Stewart and Sun from [17, Chapter VI]. From now on, let $(H, M)$ be a symmetric definite pair such that (9) holds. That is, let $X = \begin{bmatrix} X_1 & X_2 \end{bmatrix}$ be such that

$$\begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} H \begin{bmatrix} X_1 & X_2 \end{bmatrix} = \begin{bmatrix} \Lambda_1 & \Lambda_2 \\ \Lambda_2^* & \Lambda_1^* \end{bmatrix}, \quad \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} M \begin{bmatrix} X_1 & X_2 \end{bmatrix} = \begin{bmatrix} I_k & I_{n-k} \end{bmatrix},$$

(57)

where

$$\Lambda_1 = \text{diag}(\lambda_1, \ldots, \lambda_k), \quad \Lambda_2 = \text{diag}(\lambda_{k+1}, \ldots, \lambda_n),$$

and $X_1 \in \mathbb{C}^{n \times k}$, $X_2 \in \mathbb{C}^{n \times n-k}$. The following theorem contains a bound for the Frobenius norm of the diagonal matrix which contains the sines of the canonical angles between eigenspace $\text{Ran}(X_1)$ and corresponding perturbed eigenspace $\text{Ran}(\tilde{X}_1)$.

\footnote{Here we have tacitly used the Matlab notation to define the matrix $M$.}
Theorem 4.1 (Sun). Let the definite pair \((H, M)\) be decomposed as in (57), where \(X_1\) and \(X_2\) have orthonormal columns. Let the analogous decomposition be given for the pair \((\tilde{H}, \tilde{M})\equiv (H+\delta H,M+\delta M)\) and let \(\lambda_i\) and \(\tilde{\lambda}_i\), \(i = 1, \ldots, n\) be used — assuming the ordering of eigenvalues as in (9) — to denote the eigenvalues of \((H, M)\) and \((\tilde{H}, \tilde{M})\) respectively. If

\[
\min \left\{ \frac{|\tilde{\lambda}_j - \lambda_i|}{\sqrt{(1 + \tilde{\lambda}_j^2)(1 + \lambda_i^2)}} ; i = 1, \ldots, k, j = k + 1, \ldots, n \right\} > 0, \\
\min_{x \in \mathbb{C}^n} \frac{\sqrt{(x^*Hx)^2 + (x^*Mx)^2}}{\|x\| = 1} > 0
\]

then

\[
\| \sin \Theta (\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \|_F \leq \frac{\sqrt{\|H^2 + M^2\|} \sqrt{\|\delta H X_1\|_F^2 + \|\delta M X_1\|_F^2}}{\gamma(H, M) \gamma(\tilde{H}, M) \Gamma},
\]

where

\[
\gamma(H, M) = \min_{x \in \mathbb{C}^n} \sqrt{(x^*Hx)^2 + (x^*Mx)^2} > 0,
\]

is called the Crawford number of the pencil \(H - \lambda M\) (see for example [7, Section 8.7] or [17, Section VI 1.3]) and

\[
\Gamma = \min \left\{ \frac{|\tilde{\lambda}_j - \lambda_i|}{\sqrt{(1 + \tilde{\lambda}_j^2)(1 + \lambda_i^2)}} ; i = 1, \ldots, k, j = k + 1, \ldots, n \right\}
\]

is an absolute measure of the gap in the spectrum.

Experiment 4.2. We estimate the perturbation of an invariant subspace which corresponds to the first four smallest eigenvalues of the matrix pair \((H, M)\). The experiment is to be understood in the context of testing of the asymptotic sharpness of the effectivity quotients. Step1: Measuring the performance of our estimate. The exact perturbation gives:

\[
\| \sin \Theta_M (\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \approx 6.727 \cdot 10^{-7}.
\]

For the constants which describe the spectral configuration for Theorem 3.2 as given by condition (32) we have

\[
\alpha = 3.4363 \cdot 10^{-4}, \quad \delta = 5.9898 \cdot 10^{-6}.
\]

Further, the quantities \(\eta_H \equiv \|H^{-1/2}\delta HH^{-1/2}\|\) and \(\eta_M \equiv \|M^{-1/2}\delta MM^{-1/2}\|\) are bounded by

\[
\eta_H \leq 5.9 \cdot 10^{-8}, \quad \eta_M \leq 10^{-8}.
\]
Now using the above, bound (47) yields

\[ \| \sin \Theta_M(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \| \leq 4.1 \cdot 10^{-6}. \]

**Step 2: Measuring the performance of the Stewart-Sun bound.** Bound (58) is not satisfactory for this example due the fact that \( \gamma(H, M) = 1 \), and \( \gamma(H + \delta H, M + \delta M) \approx 1 + \eta \). On the other hand, the gap \( \Gamma \sim 10^{-6} \) and \( \sqrt{\|H^2 + M^2\|} \sim 10^5 \). Note that \( \Gamma = \delta \) for \( \delta \) from (60). Together with \( \sqrt{\|\delta HX_1\|_F^2 + \|\delta MX_1\|_F^2} = 10^{-8} \), we have that (58) gives

\[ \| \sin \Theta(\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)) \|_F \leq 6 \cdot 10^5. \]

### 4.1.2. Asymptotic behavior of the parameter dependent family of problems for the CYL-SHELL problem

For some \( n \in \mathbb{N} \) let \( X_n \in \mathbb{R}^{5489 \times 2} \), \( X^*_nX_n = I_2 \) by an orthogonal matrix. We define the matrix \( \delta H_n \) by the Kahan’s formula

\[ \delta H_n = R_nX^*_n + X_nR^*_n, \]

where \( R_n = HX_n - X_n(X^*_nHX_n) \) is the residual matrix. We compute singular values \( s_1(n) \leq s_2(n) \) of the matrix

\[ \tilde{H}_n^{-1/2}(H - \tilde{H}_n)\tilde{H}_n^{-1/2}X_n = \tilde{H}_n^{-1/2}\delta H_n\tilde{H}_n^{-1/2}X_n \]

using the variational characterization\(^5\) from [9]. With this notation we have \( \eta_{\tilde{H}_n} = s_2(n) \), and we can use both \( s_1(n) \) and \( s_2(n) \) to compute other unitary invariant norms of \( \tilde{H}_n^{-1/2}(H - \tilde{H}_n)\tilde{H}_n^{-1/2} \) if needed.

Note that the matrix \( \tilde{H}_n \) has the eigenvalues of the so called generalized Rayleigh quotient \( X^*_nHX_n \) in its spectrum. The associated eigenvectors are contained in the column subspace of \( X_n \).

**Experiment 4.3.** Let now \( U_1 \in \mathbb{R}^{5489 \times 2} \), \( U^*_1U_1 = I_2 \) be such that \( \text{Ran}(U_1) \) is the invariant subspace associated with the two lowermost eigenvalues of \( H \). The results of this paper allow us to estimate both the subspace approximation error \( \sin \Theta(X_1, U_1) \) as well as \( \sin \Theta_H(X_1, U_1) \) in terms of \( \eta_{\tilde{H}_1} \). In the first case, we consider the matrix pair \( (H, I) \), whereas in the second case we can consider \( (I, H) \).

We will now consider a particular parameter dependent sequence of orthogonal matrices \( X_n \). Let \( T = \begin{bmatrix} T_1 & 0 \end{bmatrix}^* \in \mathbb{C}^{5489 \times 2} \), where \( T_1 \) is a random \( 2 \times 2 \) matrix. We compute the sequence of orthogonal matrices \( X_n \), where \( \text{Ran}(X_n) = \text{Ran}(U_1 + \frac{1}{1+n}T) \).

---

\(^5\)Singular values \( s_1(n) \) and \( s_2(n) \) can be computed or estimated efficiently by e.g. using approximations of the matrix moment problem or by the use of hierarchical preconditioners cf. [9].
In each step we compute and plot the following quotients

\[ q_n^{\text{eu}} = \frac{\| \sin(\text{Ran}(X_n), \text{Ran}(U_1)) \|}{\eta_{\tilde{H}_n}} \quad q_n^H = \frac{\| \sin_H(\text{Ran}(X_n), \text{Ran}(U_1)) \|}{\eta_{\tilde{H}_n}}. \]

The quotients \( q_n^{\text{eu}} \) is denoted with \(*\) and \( q_n^H \) with the solid line in Figure 2. When defining these effectivity quotients we have ignored the measures of the gap. This does not affect the analysis of the problem, since the measures of the gap converge to a fixed positive number as \( \eta_{\tilde{H}_n} \to 0 \) and so do not influence the asymptotic behavior of the effectivity quotient.

\[ \begin{align*}
\text{Figure 2: Effectivity for parameter dependent perturbations. The effectivity }& q_n^{\text{eu}} \text{ drops like } O(\frac{1}{1+n}), \text{ whereas we observe } q_n^H = O(1). \text{ Note that this can be proved formally by computing the analytic expansions for the perturbation of the spectral projections of the operators } \\
\eta_{\tilde{H}_n} & \text{ appears to be too pessimistic estimator of } \sin \Theta(\text{Ran}(X_n), \text{Ran}(U_1)), \text{ whereas it is an asymptotically sharp estimator of } \sin \Theta_H(\text{Ran}(X_n), \text{Ran}(U_1)).
\end{align*} \]

5. Conclusion

In this paper we have produced new bounds for the rotation of the eigenspaces of a Hermitian positive definite matrix pair. The experiments from Section 4.1.2 show that \( \eta_H \) is a sharp estimator of the size of the rotation in the \( H \) dependent scalar product, whereas it can be an overly pessimistic estimator of the size of the rotation in the Euclidean scalar product. In fact, in Appendix A we present an example where \( \eta_H \) is an asymptotically sharp estimator of the rotation angle.

This type of the performance of the effectivity quotient is characteristic for parameter dependent model problems. Let us point out that our theory is particularly suitable for analyzing model problems with ill conditioned matrices. In Section 4 we considered model
problems where the ill conditioning was induced by the fact that the matrices were discretizations of unbounded operators in a Hilbert space, cf. Appendix A for another class of examples.

In our future work we plan to extend this analysis to include matrices where null spaces are present and the question of the choice of an appropriate matrix norm is central.

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References


Appendix A. A simple penalty type eigenvector perturbation

Motivation for the Appendix. The purpose of Appendix A is to illustrate the applicability of our estimates on a family of perturbations which are introduced by the presence of a large penalty parameter in the model. We first present a general discussion, which can be seen as an eigenvector analogon of the eigenvalue results from [18]. We then proceed to present a simple completely soluble academic model problem and show that our estimator is asymptotically sharp on this example.

Many differential problems with algebraic constraints such as Stokes or Maxwell systems can be discretized in the generic block matrix form like

$$H_\kappa = \begin{bmatrix} L_b & R_b^* \\ R_b & C_b \end{bmatrix} + \kappa \begin{bmatrix} 0 & 0 \\ 0 & H_e \end{bmatrix}. \quad (A.1)$$

We assume here that the matrix $H_\kappa$ is Hermitian positive definite and that $L_b$, $C_b$ and $H_e$ are also Hermitian positive definite matrices. By setting $\kappa$ large, an algebraic constraint is imposed on the system described by the matrix $H_\kappa$ which can be observed as an implicit block diagonalization of the matrix $H_\kappa$.

This can be best expressed by asymptotic expressions like (3) and (4) from Section 1. By

$$\bar{H}_\kappa = \begin{bmatrix} L_b \\ C_b + \kappa H_e \end{bmatrix}$$
we denote the block diagonal of $H_\kappa$ and compute
\[
\|\tilde{H}_\kappa^{-1/2}(\tilde{H}_\kappa - H_\kappa)\tilde{H}_\kappa^{-1/2}\| = \left\| \begin{bmatrix} 0 & L_b^{-1/2}R_b^* (C_b + \kappa H_\epsilon)^{-1/2} \\ (C_b + \kappa H_\epsilon)^{-1/2}R_bL_b^{-1/2} & 0 \end{bmatrix} \right\| \\
= \frac{1}{\sqrt{\kappa}} \left\| \begin{bmatrix} 0 & \frac{L_b^{-1/2}R_b^* (\frac{1}{\kappa} C_b + H_\epsilon)^{-1/2}}{\kappa} \\ (\frac{1}{\kappa} C_b + H_\epsilon)^{-1/2}R_bL_b^{-1/2} & 0 \end{bmatrix} \right\| \\
= O\left(\frac{1}{\sqrt{\kappa}}\right).
\]

Let us introduce the perturbation estimate $\eta_{\tilde{H}_\kappa} := \|\tilde{H}_\kappa^{-1/2}(\tilde{H}_\kappa - H_\kappa)\tilde{H}_\kappa^{-1/2}\|$. The positive definiteness of $H_\kappa$ implies that $\eta_{\tilde{H}_\kappa} < 1$ for every $\kappa > 1$. With this we note the following inequalities
\[
|x^*H_\kappa x - x^*\tilde{H}_\kappa x| \leq \eta_{\tilde{H}_\kappa} x^*\tilde{H}_\kappa x, \quad x \in \mathbb{C}^n, \quad (A.2)
\]
\[
|x^*H_\kappa^{-1} x - x^*\tilde{H}_\kappa^{-1} x| \leq \frac{\eta_{\tilde{H}_\kappa}}{1 - \eta_{\tilde{H}_\kappa}} x^*\tilde{H}_\kappa^{-1} x, \quad x \in \mathbb{C}^n. \quad (A.3)
\]

Obviously, with this analysis we can choose
\[
\eta_{H_\kappa^{-1}} = \frac{\eta_{\tilde{H}_\kappa}}{1 - \eta_{\tilde{H}_\kappa}} \quad (A.4)
\]
and so we can apply Theorem 3.5 directly to the matrix pairs $(H_\kappa, I)$, $(I, H_\kappa)$, $(H_\kappa^{-1}, H_\kappa)$ and $(I, H_\kappa^{-1})$. These matrix pairs are interesting because they have the same eigenvectors as the matrix $H_\kappa$. By considering them we obtain estimates of the eigenvector rotation for the matrix $H_\kappa$ induced by the large penalty parameter $\kappa$ in the Euclidean scalar product, $H_\kappa$-dependent scalar product and $H_\kappa^{-1}$-dependent scalar product. In the case when $H_\kappa$ is a discretization of a differential operator, these scalar products are discrete variants of the scalar products in the associated positive and negative order Sobolev spaces. In what follows we will be interested in the estimates of the rotation of eigenvectors in the $H_\kappa$ dependent scalar product. To this end we will concentrate on the matrix pair $(H_\kappa^{-1}, H_\kappa)$.

The behavior of the spectra of the family of problems (A.7) has been analyzed in [18] with the help of the Gerschgorin theorem. There the authors start by writing the implicit partial diagonalization of $H_\kappa$ in the generic block matrix form
\[
\begin{bmatrix} L_b & R_b^* \\ R_b & C_b + \kappa H_\epsilon \end{bmatrix} \begin{bmatrix} V_\kappa \\ W_\kappa \end{bmatrix} = \begin{bmatrix} V_\kappa \\ W_\kappa \end{bmatrix} \Lambda_\kappa, \quad (A.5)
\]
where $L_b$, $C_b$, $R_b$ and $H_\epsilon$ are as in (A.1) and $\Lambda_\kappa$ is the diagonal matrix containing the targeted eigenvalues. The orthogonality property $V_\kappa^*V_\kappa + W_\kappa^*W_\kappa = I$ together with the Gerschgorin theorem implies, the estimates
\[
\|L_b V_\kappa - V_\kappa \Lambda_\kappa\| = O\left(\frac{1}{\kappa}\right), \quad \|V_\kappa^* V_\kappa - I\| = O\left(\frac{1}{\kappa^2}\right), \quad \|W_\kappa\| = O\left(\frac{1}{\kappa}\right), \quad (A.6)
\]
see [18, p. 3209]. In the example that follows we show this explicitly on a model problem and indicate a possible dependence on $\kappa$ of the otherwise unaccessible matrix $V_\kappa$. 

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Appendix A.1. A simple numerical example

Although we can technically treat the case of a general block matrix, it is illustrative to consider the following explicit family of matrices

$$H_\kappa = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 + \kappa \end{bmatrix}, \quad \kappa \gg 1. \tag{A.7}$$

By $\lambda_1 < \lambda_2 < \lambda_3$ we denote the eigenvalues of $H_\kappa$. For eigenvectors we also use the following notation

$$H_\kappa v^\kappa_i = \lambda^\kappa_i v^\kappa_i, \quad i = 1, 2, 3.$$ 

These eigenvalues and eigenvectors can be given explicitly as functions of $\kappa$

$$\begin{align*}
\lambda_1^\kappa &= 1 - \frac{1}{2\kappa} + \frac{3}{8\kappa^2} - \frac{55}{128\kappa^4} + \frac{1}{2\kappa^5} + O\left(\frac{1}{\kappa^6}\right) \\
\lambda_2^\kappa &= 3 - \frac{1}{2\kappa} - \frac{3}{8\kappa^2} + \frac{55}{128\kappa^4} + \frac{1}{2\kappa^5} + O\left(\frac{1}{\kappa^6}\right) \\
\lambda_3^\kappa &= \kappa + 2 + \frac{1}{\kappa} - \frac{1}{\kappa^3} + O\left(\frac{1}{\kappa^5}\right)
\end{align*}$$

$$\begin{align*}
v_1^\kappa &= \begin{bmatrix} 1 + \frac{1}{2\kappa} + \frac{5}{8\kappa^2} - \frac{1}{2\kappa^3} - \frac{7}{128\kappa^4} + \frac{1}{2\kappa^5} - \frac{675}{1024\kappa^6} + O\left(\frac{1}{\kappa^7}\right) \\
1 + \frac{3}{8\kappa^2} + \frac{55}{128\kappa^4} - \frac{1}{2\kappa^5} + O\left(\frac{1}{\kappa^6}\right) \\
1 - \frac{1}{\kappa} + \frac{1}{2\kappa^2} + \frac{3}{8\kappa^3} - \frac{55}{128\kappa^5} - \frac{1}{2\kappa^6} + O\left(\frac{1}{\kappa^7}\right) \end{bmatrix}, \\
v_2^\kappa &= \begin{bmatrix} \left(\frac{1}{\kappa}\right)^2 - \left(\frac{1}{\kappa}\right)^4 + O\left(\frac{1}{\kappa^4}\right) \\
-\frac{1}{\kappa} + \left(\frac{1}{\kappa}\right)^5 + O\left(\frac{1}{\kappa^5}\right) \\
1 \end{bmatrix}, \\
v_3^\kappa &= \begin{bmatrix} \left(\frac{1}{\kappa}\right)^2 - \left(\frac{1}{\kappa}\right)^4 + O\left(\frac{1}{\kappa^4}\right) \\
-\frac{1}{\kappa} + \left(\frac{1}{\kappa}\right)^5 + O\left(\frac{1}{\kappa^5}\right) \\
1 \end{bmatrix}
\end{align*}$$

and $\eta_{\bar{H}_\kappa} = \sqrt{\frac{2}{6 + 3\kappa}}$. Note that the matrix $\left[V_\kappa \; \hat{W}_\kappa\right]^*$ has columns given by $v_1^\kappa$ and $v_2^\kappa$, and so in this example we can see the dependence $V_\kappa$ on the penalty parameter explicitly.

Using (A.4) we obtain for the pair $(H^{-1}_\kappa, H_\kappa)$ the right hand side

$$\text{Right}(\kappa) := 3\kappa \frac{\eta_{H^{-1}_\kappa}}{\kappa^2 - 3^2} \frac{\eta_{H^{-1}_\kappa}}{\sqrt{1 - \eta_{H^{-1}_\kappa}}} + \kappa^2 \frac{\eta_{\bar{H}_\kappa}}{\kappa^2 - 3^2} \frac{\eta_{\bar{H}_\kappa}}{\sqrt{1 - 2\eta_{\bar{H}_\kappa}}} = O\left(\frac{1}{\sqrt{\kappa}}\right). \tag{A.8}$$

as the estimator for the Left$(\kappa) := \sin \Theta_{H_\kappa}(\text{Ran}[v_1^\kappa \; v_2^\kappa], \text{Ran}[v_1^\infty \; v_2^\infty])$. Since we also have an explicit formula for $v_i^\kappa$, we can compute the effectivity quotient $\text{Right}(\kappa)/\text{Left}(\kappa)$ for this particular example and obtain

$$\lim_{\kappa \to \infty} \frac{\text{Left}(\kappa)}{\text{Right}(\kappa)} = 1.$$
Here we have used the symbol $v_i^\infty$, $i = 1, 2, 3$ to denote the limit eigenvectors of $v_i^\kappa$, $i = 1, 2, 3$ as $\kappa \to \infty$. They are also the eigenvectors of the limit matrix

$$H_\infty = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$ 

This shows that the energy norm estimate is sharp when viewed as the function of $\kappa$. On the other hand a simple computation reveals that any of the sin $\Theta$ theorems from [5, 10, 15] yields a similar $O(\frac{1}{\sqrt{\kappa}})$ — or even less sharp\(^6\) $O(1)$ — upper estimate for the

$$\sin \Theta(\text{Ran}[v_1^\kappa v_2^\kappa], \text{Ran}[v_1^\infty v_2^\infty]) = O(\frac{1}{\kappa}).$$

Furthermore, although we have a $3 \times 3$ matrix example, Theorem 4.1 cannot be used — because $\|\delta H_\kappa\| \to \infty$ as $\kappa \to \infty$ — to follow the rotation to the limit in $\kappa$.

This shows that a notion of the sharpness (a sin $\Theta$ theorem is considered to be sharp if there is a perturbation in the allowed class of perturbations such that the bound is attained) for the estimates of the rotation of eigenvectors is a delicate question.

Appendix A.2. Conclusion for the Appendix

A formula, similar to (A.8), can be obtained for the block matrix from (A.5). Let us assume that $\kappa$ is so large that the part of the spectrum of $H_\kappa$ which converges to the eigenvalues of $H_\infty$ is separate from the spectrum that diverges to $\infty$. We obtain an asymptotically sharp estimate of the rotation of the eigenspaces of $H_\kappa$ under the influence of the penalty parameter in the $H_\kappa$ dependent scalar product. This is our companion result to the eigenvalue Gerschgorin type argument from [18].

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\(^6\)The sharpness of the residual estimate (A.6) deteriorates when we chose an orthonormal basis for $\text{Ran}[v_1^\infty v_2^\infty]$ as the columns of $V_\kappa$ are not orthonormal.