Approximate eigenvectors as preconditioner*

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Abstract

Given approximate eigenvector matrix $\tilde{U}$ of a Hermitian nonsingular matrix H, the spectral decomposition of H can be obtained by computing $H' = \tilde{U}^* H \tilde{U}$ and then diagonalizing H'. This work addresses the issue of numerical stability of the transition from H to H' in finite precision arithmetic. Our analysis, performed in terms of so called relative errors, shows that the accuracy of the eigensolution is ensured if the approximate eigenvectors are (i) sufficiently orthonormal and (ii) the computed matrix H' is diagonal enough. In that case, H' can be efficiently and accurately diagonalized by the Jacobi method. If $\tilde{U}$ is computed by fast eigensolver based on tridiagonalization, this procedure usually gives the eigensolution with high relative accuracy and it is more efficient than accurate Jacobi type methods pure.

1 Introduction

If $\tilde{U}$ is an approximate matrix of eigenvectors of a Hermitian matrix H, then the *preconditioned* matrix

$$H' = \tilde{U}^* H \tilde{U} \tag{1}$$

is expected to be nearly diagonal. As a consequence, one would expect that the matrix H' will be better accessible to the eigenvalue analysis in the sense that its eigenvalue problem will be solvable more quickly and more accurately. The source for $\tilde{U}$ may be manifold. For instance, $\tilde{U}$ may be the eigenvector matrix of a neighbor problem in course of a parameter analysis, or just eigenvectors computed by a fast but less accurate method. The product (1) may also come in forming the Ritz approximation of H in a given subspace, in this case $\tilde{U}$ will contain not all approximate eigenvectors, but a selection of them. For some other important instances with preconditioning see [21]. The aim of this paper is to investigate numerical feasibility of the preconditioning (1) and its applications in various settings.

The first task is to analyze computation of (1) which, in finite precision arithmetic, may lead to an $H' + \delta H'$ with eigenvalues too far from the ones of H. In this paper we use the relative distance $|\delta\lambda_i/\lambda_i|$ to measure the accuracy of approximating an eigenvalue λ_i of H with $\lambda_i + \delta\lambda_i$, $i = 1, \ldots, n$. This type of accuracy cannot be analyzed using the classical perturbation theory. To illustrate, let δH be Hermitian perturbation of H such that $|\delta H| \leq \varepsilon |H|$, where the matrix absolute values and matrix inequality are understood element–wise. In the classical theory, we use Weyl's theorem and the inequality $\|\delta H\|_2 \leq n\varepsilon \|H\|_2$ to obtain

$$|\delta\lambda_i| \leq n\varepsilon \|H\|_2, \quad \frac{|\delta\lambda_i|}{|\lambda_i|} \leq n\varepsilon\kappa_2(H), \quad \text{where } \kappa_2(H) = \|H\|_2 \|H^{-1}\|_2. \tag{2}$$

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This estimate gives pessimistic relative error bound for λ_i with $|\lambda_i| \ll \|H\|_2$. In other words, the bound (2) gives no guarantee for the accuracy of small eigenvalues λ_i, which are often the most important ones.

On the other hand, there are several important classes of Hermitian matrices for which all eigenvalues are well determined by matrix entries: small element–wise rounding errors ($|\delta H| \leq \boldsymbol{\varepsilon}|H|$) cause only small relative errors $|\delta\lambda_i|/|\lambda_i|$, $1 \leq i \leq n$, independent of the size of $\kappa_2(H)$. Such matrices are colloquially called *well behaved*. Barlow and Demmel [2] show that scaled diagonally dominant matrices are well behaved. (Recall that scaled diagonally dominant matrices (γ–s.d.d.) are characterized by the factorization $H = D(J+N)D$, where $D = \mathrm{diag}(|H_{ii}|)^{1/2}$, $|J| = I$ and $\|N\|_2 \leq \gamma < 1$.) Demmel and Veselić [3] show that a positive definite matrix H is well behaved if and only if in the factorization $H = DH_sD$ with $D = \mathrm{diag}(H_{ii})^{1/2}$, the value of $\|H_s^{-1}\|_2$ is moderate. Veselić and Slapničar [25] describe a new class of well behaved Hermitian (symmetric) matrices and give a perturbation theory that includes the previous analyses of scaled diagonally dominant matrices and positive definite matrices. All these results are applications of the following general theorem.

Theorem 1.1 *(Veselić and Slapničar [25]) Let H be a Hermitian matrix and $\lceil H \rceil = \sqrt{H^2}$. Let δH be Hermitian perturbation of H such that for some $\eta \in [0,1)$*

$$|x^*\delta H x| \leq \eta x^* \lceil H \rceil x, \quad x \in \mathbf{C}^n \tag{3}$$

holds. Then the distance between each eigenvalue λ of H and its matching eigenvalue $\lambda + \delta\lambda$ of $H + \delta H$ is bounded by

$$|\delta\lambda| \leq \eta|\lambda|. \tag{4}$$

Note that from the spectral decomposition $H = U\Lambda U^*$ of H it follows that $\lceil H \rceil = U|\Lambda|U^*$ and that for all i, j $|H_{ij}| \leq \sqrt{\lceil H \rceil_{ii}\lceil H \rceil_{jj}}$. Furthermore, it is shown in [25] that H is well behaved if $\lceil H \rceil$ is *well scaled*, that is if in the factorization

$$\lceil H \rceil = \mathrm{diag}(\lceil H \rceil_{ii})^{1/2} \lceil H \rceil_s \mathrm{diag}(\lceil H \rceil_{ii})^{1/2}$$

the value of $\|\lceil H \rceil_s^{-1}\|_2$ is moderate. More precisely, if in Theorem 1.1 $|\delta H| \leq \boldsymbol{\varepsilon}|H|$, or more generally, if $|\delta H_{ij}| \leq \boldsymbol{\varepsilon}\sqrt{\lceil H \rceil_{ii}\lceil H \rceil_{jj}}$, then the estimate (4) holds with $\eta \leq n\boldsymbol{\varepsilon}\|\lceil H \rceil_s^{-1}\|_2$. To compare this bound with the classical one (2), note that $\kappa_2(\lceil H \rceil_s) \leq n\kappa_2(\lceil H \rceil) = n\kappa_2(H)$, and that it is possible that $\kappa_2(\lceil H \rceil_s) \ll \kappa_2(H)$.

The fastest known method that achieves high relative accuracy on well scaled matrices is the Jacobi method [13], [14]. Rigorous perturbation analyses of Demmel and Veselić [3], Drmač [5], [7], Mathias [18] show that on positive definite matrices the relative error in the computed eigenvalues is less than $\wp(n)\mathbf{u}\|H_s^{-1}\|_2$, where $\wp(n)$ is modest polynomial. If the matrix is indefinite, the standard Jacobi method generally lacks the high relative accuracy and has to be modified as follows: using suitable pivoting, compute the symmetric indefinite factorization $\pi^\tau H \pi = GJG^*$ ($J = \mathrm{diag}(\pm 1)$) and solve the equivalent problem of diagonalization of definite matrix pencil $G^*G - \lambda J$, using the J–symmetric Jacobi algorithm due to Veselić [24]. A rigorous analysis that demonstrates the accuracy of this algorithm is due to Slapničar [22]. However, if the matrix is sufficiently scaled diagonally dominant, even the classical Jacobi method is accurate. There is yet no rigorous error analysis confirming this well established numerical evidence. This will be the subject for a future research.

Another application of the Jacobi method as cleanup is in solving a sequence of eigenvalue problems of several close Hermitian matrices. In that case, $\tilde{U}$ is known approximation of the eigenvector matrix of some H_0 that is close to H ($\|H - H_0\|_2 \ll \|H\|_2$, say) and we expect that the matrix $\tilde{U}^*H\tilde{U}$ will be closer to diagonal form than H is. Hence, it seems reasonable to start the diagonalization process with the preconditioning transformation $H \mapsto H' = \tilde{U}^*H\tilde{U}$. If the off–diagonal part of H' is sufficiently small, the eigendecomposition of H can be efficiently and accurately completed with the Jacobi method applied to H'. In this case, the Jacobi method is a natural choice because of its simplicity, fast convergence on almost diagonal matrices, and because of its accuracy.

In order to apply the idea of preconditioning $H \mapsto H' = \tilde{U}^* H \tilde{U}$ followed by iterative improvement with confidence in the practice, several theoretical issues need to be addressed first. In this paper, we restrict our attention to the preconditioning step. (An analysis of the iterative improvement is the subject of our future work.) In § 2, we give detailed error and perturbation analyses of floating–point transformation (5). We show that on well–scaled matrices the preconditioning step is accurate provided that $\tilde{U}$ is reasonable approximation of the eigenvectors of H. We analyse the diagonal structure of the preconditioned matrix and we also discuss the possibility of using approximate singular values of H as preconditioner. Our estimates are accompanied with illustrative numerical examples. In § 3, we analyse the structure of the spectral absolute value $\lvert H \rvert$ of an s.d.d. matrix H. The analysis shows that taking the spectral absolute value does not worsen the diagonal dominance of the matrix H. In § 4, we show that using fast matrix multiplication algorithms is not feasible in the computation of $H' = \tilde{U}^* H \tilde{U}$ because of a potential loss of accuracy and because the overall speedup in solving the diagonalization problem is almost negligible. In § 5 we present some numerical illustrations showing that our algorithm mostly improves the accuracy of the fast methods while taking less time than the Jacobi methods pure.

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2 Analysis of the preconditioning

The preconditioning replaces the original matrix H by

$$\tilde{H}' = \tilde{U}^* H \tilde{U} + \delta H', \tag{5}$$

where $\tilde{U}$ are the approximate eigenvectors. Before we give eigenvalue perturbation estimates for the matrix $\tilde{H}'$ in the relation (5), let us briefly describe the perturbation $\delta H'$ in (5). Consider first the real case. Real floating–point matrix computation using the standard algorithms is denoted by $\mathtt{fl}_r(\cdot)$. The product $H\tilde{U}$ is approximated by $\mathtt{fl}_r(H\tilde{U}) = H\tilde{U} + \mathcal{E}_1$. To ensure symmetry and to save unnecessary computation only the upper triangle of $\mathtt{fl}_r(\tilde{U}^\tau \mathtt{fl}_r(H\tilde{U}))$ is computed. If the whole matrix is needed, the strictly upper triangle is transposed and copied into the strictly lower triangle. It holds $\mathtt{fl}_r(\tilde{U}^\tau \mathtt{fl}_r(H\tilde{U})) = \tilde{U}^\tau(H\tilde{U} + \mathcal{E}_1) + \mathcal{E}_2$. In the case of the standard algorithm we have $|\mathcal{E}_1| \le \mathbf{u}_P |H| \cdot |\tilde{U}|$ and

$$|\mathcal{E}_2| \le \mathbf{u}_P |\tilde{U}^\tau| \cdot (|H\tilde{U}| + \mathbf{u}_P |H| \cdot |\tilde{U}|), \quad |\tilde{U}^\tau \mathcal{E}_1| \le \mathbf{u}_P |\tilde{U}^\tau| \cdot |H| \cdot |\tilde{U}|,$$

where

$$\mathbf{u}_P \le n\mathbf{u} + O(\mathbf{u}^2). \tag{6}$$

Hence, we obtain the relation of the type (5):

$$\tilde{H}' = \tilde{U}^* H \tilde{U} + \delta H', \quad |\delta H'| \le \boldsymbol{\varepsilon} |\tilde{U}|^\tau \cdot |H| \cdot |\tilde{U}|, \;\; \boldsymbol{\varepsilon} = 2\mathbf{u}_P + O(\mathbf{u}^2). \tag{7}$$

Remark 2.1 The relation (6) can for $n < 1/\mathbf{u}$ be replaced by $\mathbf{u}_P \le \mathbf{u} + O(\mathbf{u}^2)$ if we use double precision accumulation in computing the inner products.

Remark 2.2 Unfortunately, the BLAS 3 library [4] does not contain a procedure that can take advantage of the symmetry of the final matrix product. Thus, the complexity of computing $\tilde{H}'$ using BLAS 3 is $4n^3 + O(n^2)$ *flops*. This cost can be reduced in a BLAS based implementation as follows. Write H as

$$H = H_\triangleright + (H_\triangleright)^\tau, \quad (H_\triangleright)_{ij} = \begin{cases} H_{ij}, & i < j, \\ \frac{1}{2} H_{ii}, & i = j, \\ 0, & i > j, \end{cases}$$

and note that $U^\tau H U = (U^\tau H_\triangleright U) + (U^\tau H_\triangleright U)^\tau$. The trick is that $H_\triangleright U$ can be computed in $n^3 + O(n^2)$ *flops* using BLAS 3 procedure `STRMM()`. This reduces the total cost to $3n^3 + O(n^2)$ *flops*. Error analysis is similar to the one above if we note that $|H| = |H_\triangleright| + |H_\triangleright|^\tau$.

Consider now complex $H = H_r + \mathbf{i}H_i$ and almost unitary $\tilde{U} = \tilde{U}_r + \mathbf{i}\tilde{U}_i$, where H_r, H_i, $\tilde{U}_r$, $\tilde{U}_i$ are real matrices. If complex multiplication $\mathtt{fl}_c(\cdot)$ is defined by

$$\mathtt{fl}_c(H\tilde{U}) = \mathtt{fl}_r(H_r\tilde{U}_r - H_i\tilde{U}_i) + \mathbf{i}\,\mathtt{fl}_r(H_r\tilde{U}_i + H_i\tilde{U}_r),$$

then it immediately follows that $|\mathtt{fl}_c(H\tilde{U}) - H\tilde{U}| \leq 2(n+1)\mathbf{u}|H|\cdot|\tilde{U}|$. Hence, $\mathtt{fl}_c(\tilde{U}^*\mathtt{fl}_c(H\tilde{U}))$ satisfies a relation similar to (7). A similar conclusion holds if H and $\tilde{U}$ are stored in two $n \times n$ complex arrays and if $\mathtt{fl}_c(\cdot)$ is defined in a standard way, using complex scalar arithmetic.
In our first estimate, we follow the usual backward analysis approach. Our basic assumption is that the matrix H is well scaled, that is, the value of $\|{\lvert H \rvert}_s^{-1}\|_2$ is moderate.

Theorem 2.1 *(Backward analysis.) Let $H \in \mathbf{C}^{n\times n}$ be a Hermitian nonsingular matrix, $\tilde{U}$ an almost unitary matrix with $\nu \equiv \|\tilde{U}^*\tilde{U} - I\|_2 < 1$, and let $\tilde{H}'$ be defined as in the relation (7). Furthermore, let $\lvert H \rvert = \Delta \lvert H \rvert_\Delta \Delta$, $H = \Delta H_\Delta \Delta$, $\tilde{U}^*\lvert H \rvert\tilde{U} = \Xi X_\Xi \Xi$, where Δ and Ξ are diagonal positive definite matrices. If $\lambda_1 \geq \cdots \geq \lambda_n$ and $\tilde{\lambda}'_1 \geq \cdots \geq \tilde{\lambda}'_n$ are the eigenvalues of H and $\tilde{H}'$, respectively, then*

$$\tilde{\lambda}'_i = \lambda_i(1+\theta_i)(1+\theta'_i), \quad 1 \leq i \leq n, \tag{8}$$

where, for all $1 \leq i \leq n$, $|\theta'_i| \leq \nu$,

$$|\theta_i| \leq \boldsymbol{\varepsilon} \inf_{\Delta} \|\, \lvert H \rvert_\Delta^{-1} \,\|_2 \|\, |H_\Delta| \,\|_2 \;\inf_{\Xi} \mathrm{Trace}(\|X_\Xi^{-1}\|_2 X_\Xi), \tag{9}$$

provided that the right hand side in (9) is less than one.

<u>**Proof**</u> First, we rewrite the relation $\tilde{H}' = \tilde{U}^* H \tilde{U} + \delta H'$ as

$$\tilde{H}' = \tilde{U}^*(H + \tilde{U}^{-*}\delta H'\tilde{U}^{-1})\tilde{U} = \tilde{U}^*(H + \delta H)\tilde{U}, \tag{10}$$

where we define $\delta H = \tilde{U}^*\delta H'\tilde{U}^{-1}$. Next, we compare the eigenvalues of H and $H + \delta H$. Denote the later (non–increasingly ordered) as $\lambda_i + \delta\lambda_i$, $1 \leq i \leq n$. We know that $|\delta\lambda_i|/|\lambda_i|$, $1 \leq i \leq n$, are small if $\|\, \lvert H \rvert^{-1/2}\delta H \lvert H \rvert^{-1/2} \,\|_2$ is small. More precisely,

$$\|\, \lvert H \rvert^{-1/2}\delta H \lvert H \rvert^{-1/2} \,\|_2 \leq \eta \;\text{ implies }\; \sup_{x\neq \mathbf{0}} \frac{|x^*\delta H x|}{x^*\lvert H \rvert x} \leq \eta,$$

and, for $\eta < 1$, Theorem 1.1 implies

$$\lambda_i + \delta\lambda_i = \lambda_i(1+\theta_i), \quad |\theta_i| \leq \eta, \quad 1 \leq i \leq n. \tag{11}$$

Now an easy calculation shows that

$$\lvert H \rvert^{-1/2}\delta H \lvert H \rvert^{-1/2} = Y^\tau(\Xi^{-1}\delta H'\Xi^{-1})Y, \quad Y = \Xi\tilde{U}^{-1}\lvert H \rvert^{-1/2}. \tag{12}$$

Note that $YY^\tau = X_\Xi^{-1}$. Hence,

$$\|\, \lvert H \rvert^{-1/2}\delta H \lvert H \rvert^{-1/2} \,\|_F \leq \|X_\Xi^{-1}\|_2 \|\Xi^{-1}\delta H'\Xi^{-1}\|_F. \tag{13}$$

Further, the relation (7) implies that

$$|\Xi^{-1}\delta H'\Xi^{-1}| \leq \boldsymbol{\varepsilon}|Z|^\tau(\Delta^{-1}|H|\Delta^{-1})|Z|$$

holds with $Z = \Delta\tilde{U}\Xi^{-1}$. Note that the obvious relation $Z^\tau |H|_\Delta Z = X_\Xi$ implies that there exists an orthogonal matrix W such that $|H|_\Delta^{1/2} Z = W X_\Xi^{1/2}$. Hence, $\| \, |Z| \, \|_F = \|Z\|_F \leq \||H|_\Delta^{-1/2}\|_2 \|X_\Xi^{1/2}\|_F$, and

$$\|\Xi^{-1}\delta H'\Xi^{-1}\|_F \leq \varepsilon \| \, |H|_\Delta^{-1} \, \|_2 \| \, |H_\Delta| \, \|_2 \|X_\Xi^{1/2}\|_F^2. \tag{14}$$

It remains to estimate the relative distance between the matching eigenvalues of $H + \delta H$ and $\tilde{H}'$. Note that the matrix $\hat{U} = \tilde{U}(\tilde{U}^*\tilde{U})^{-1/2}$ is orthogonal and that the relation (10) can be rewritten to

$$\tilde{H}' = (\tilde{U}^*\tilde{U})^{1/2}\hat{U}^*(H + \delta H)\hat{U}(\tilde{U}^*\tilde{U})^{1/2}. \tag{15}$$

Now Ostrowski's theorem [20] (or see e.g. [12]) immediately implies that for all i

$$\tilde{\lambda}_i' = (\lambda_i + \delta\lambda_i)(1 + \theta_i'), \quad |\theta_i'| \leq \|(\tilde{U}^*\tilde{U})^{1/2} - I\|_2 \leq \nu.$$

Combining this result with the estimates (11), (13) and (14) completes the proof. Q.E.D.

Remark 2.3 Note that the bound (9) is only an upper bound derived from (12) in order to reveal relevant condition numbers. More realistic bound that follows from (12) is

$$\| \, |H|^{-1/2}\delta H |H|^{-1/2} \, \|_2 \leq \varepsilon \|X_\Xi^{-1}\|_2 \|\Xi^{-1}|\tilde{U}|^\tau \cdot |H| \cdot |\tilde{U}| \cdot \Xi^{-1} \, \|_2. \tag{16}$$

Remark 2.4 To compare the result of Theorem 2.1 with the results of Mathias [18], let H be real, positive definite. The backward error analysis of the computation (7) is considered too pessimistic in [18], because the scaled backward error estimate is of the form

$$\|\Delta_H^{-1}\delta H \Delta_H^{-1}\|_2 \leq O(n^6\kappa_2^2(H_s)\mathbf{u}), \quad \Delta_H = \mathrm{diag}(H_{ii})^{1/2}, \quad H_s = \Delta_H^{-1} H \Delta_H^{-1}. \tag{17}$$

To obtain a relative error bound for the eigenvalues, the error bound in (17) is multiplied by $\|H_s^{-1}\|_2$. On the other hand, in Theorem 2.1, we scale the backward error with $|H|^{-1/2} = H^{-1/2}$ to obtain

$$\||H|^{-1/2}\delta H |H|^{-1/2}\|_2 \leq n^2\mathbf{u}\||H|_s^{-1}\|_2 \inf_\Xi \mathrm{Trace}(\|X_\Xi^{-1}\|_2 X_\Xi), \tag{18}$$

where $|H|_s = \mathrm{diag}(|H|_{ii})^{-1/2}|H|\mathrm{diag}(|H|_{ii})^{-1/2}$, and the matrix X_Ξ is expected to be close to the identity. If we use the same assumptions as in [18], then $X_\Xi = I$, and the bound in (18) becomes $n^3\mathbf{u}\|H_s^{-1}\|_2$. Finally, note that $\||H|^{-1/2}\delta H|H|^{-1/2}\|_2$ (unlike $\|\Delta_H^{-1}\delta H \Delta_H^{-1}\|_2$) bounds the relative error in the eigenvalues, and that our analysis is also valid in the case of indefinite nonsingular H.

Theorem 2.1 is "backward" in two ways. First, it follows the standard backward analysis by representing the result ($\tilde{H}'$) as a result of exact computation with perturbed data ($H+\delta H$). Second, it is backward with respect to the use of the spectral absolute value $|\cdot|$: The estimate depends on the condition of the matrix $\tilde{U}^*|H|\tilde{U}$ instead of the matrix $|\tilde{U}^*H\tilde{U}|$ or, for example, of the matrix $|\tilde{H}'|$. Of course, if $\tilde{U}$ is exactly unitary, or if H is positive definite, then $\tilde{U}^*|H|\tilde{U} = |\tilde{U}^*H\tilde{U}|$, and, in the case of almost unitary $\tilde{U}$ and indefinite H, we expect that $\tilde{U}^*|H|\tilde{U}$ is close to $|\tilde{U}^*H\tilde{U}|$. In the next theorem, we give an error bound as a function of scaled matrices $|H|$ and $|\tilde{H}'|$.

Theorem 2.2 *(Forward analysis) Let $H \in \mathbf{C}^{n\times n}$ be a Hermitian nonsingular matrix, $\tilde{U}$ an almost unitary matrix with $\nu \equiv \|\tilde{U}^*\tilde{U} - I\|_2 \ll 1$, and let $\tilde{H}'$ be defined as in the relation (7). Furthermore, let*

$$\Delta = \mathrm{diag}(|H|_{ii})^{1/2}, \quad \tilde{\Delta}' = \mathrm{diag}(|\tilde{H}'|_{ii})^{1/2}, \quad \Xi = \mathrm{diag}((\tilde{U}^*|H|\tilde{U})_{ii})^{1/2},$$

and let $|H| = \Delta|H|_s\Delta$, $H = \Delta H_s \Delta$, $|\tilde{H}'| = \tilde{\Delta}'|\tilde{H}'|_s\tilde{\Delta}'$, $\tilde{U}^\tau|H|\tilde{U} = \Xi X_s \Xi$. If $\lambda_1 \geq \cdots \geq \lambda_n$ and $\tilde{\lambda}_1' \geq \cdots \geq \tilde{\lambda}_n'$ are the eigenvalues of H and $\tilde{H}'$, respectively, then

$$\tilde{\lambda}_i' = \lambda_i \frac{1 + \theta_i'}{1 + \vartheta_i}, \quad 1 \leq i \leq n, \tag{19}$$

where, for all $1 \leq i \leq n$, $|\theta_i'| \leq \nu$,

$$|\theta_i| \leq n\varepsilon \| \lceil H \rfloor_s^{-1} \|_2 \| \lceil \tilde{H}' \rfloor_s^{-1} \|_2 \| \, |H_s| \, \|_2 \, \| \Xi \tilde{\Delta}'^{-1} \|_2^2 \tag{20}$$

and provided that the upper bound on $|\theta_i|$ *in (20) is less than one.*

Proof Define $H' = \tilde{U}^* H \tilde{U}$, and write the relation (7) as $H' = \tilde{H}' - \delta H'$. As in the proof of Theorem 2.1, we conclude that the ordered eigenvalues $\lambda_1' \geq \cdots \geq \lambda_n'$ of H' satisfy

$$\lambda_i' = \tilde{\lambda}_i'(1 + \vartheta_i), \quad 1 \leq i \leq n, \tag{21}$$

where $|\vartheta_i| \leq \| \lceil \tilde{H}' \rfloor^{-1/2} \delta H' \lceil \tilde{H}' \rfloor^{-1/2} \|_2$, $1 \leq i \leq n$. Note that by Ostrowski's theorem $\lambda_i' = \lambda_i(1 + \vartheta_i')$, $|\vartheta_i'| \leq \nu$, $1 \leq i \leq n$. Further, since for some unitary Q, $\lceil \tilde{H}' \rfloor^{-1/2} = Q \lceil \tilde{H}' \rfloor_s^{-1/2} \tilde{\Delta}'^{-1}$, we have

$$\lceil \tilde{H}' \rfloor^{-1/2} \delta H' \lceil \tilde{H}' \rfloor^{-1/2} = Q \lceil \tilde{H}' \rfloor_s^{-1/2} (\tilde{\Delta}'^{-1} \delta H' \tilde{\Delta}'^{-1}) \lceil \tilde{H}' \rfloor_s^{-1/2} Q^*,$$

and it follows that

$$|\vartheta_i| \leq \varepsilon \| \lceil \tilde{H}' \rfloor_s^{-1} \|_2 \| \tilde{\Delta}'^{-1} |\tilde{U}|^\tau \cdot |H| \cdot |\tilde{U}| \tilde{\Delta}'^{-1} \|_2, \quad 1 \leq i \leq n. \tag{22}$$

(Note that no information about $\lceil H \rfloor$ is needed in the estimate (22).) As in the proof of Theorem 2.1 we derive an upper bound for $\| \tilde{\Delta}'^{-1} |\tilde{U}|^\tau \cdot |H| \cdot |\tilde{U}| \tilde{\Delta}'^{-1} \|_2$. For the matrix $L = \tilde{\Delta}' \tilde{U}^* \Delta$ there exist an unitary matrix V such that $L^* = \lceil H \rfloor_s^{-1/2} V X_s^{1/2} \Xi \tilde{\Delta}'^{-1}$, and hence

$$\|L\|_F \leq \| \lceil H \rfloor_s^{-1/2} \|_2 \| X_s^{1/2} \|_F \| \Xi \tilde{\Delta}'^{-1} \|_2.$$

This implies the bound (20) and completes the proof. Q.E.D.

The bounds in Theorem 2.1 and Theorem 2.2 are equally good if $\tilde{U}$ is a good approximation of the eigenvector matrix U of H. Indeed, since U is the eigenvector matrix of $\lceil H \rfloor$ as well, both $\tilde{U}^* H \tilde{U}$ and $\tilde{U}^* \lceil H \rfloor \tilde{U}$ are close to diagonal matrices (in the scaled sense) and the bounds are dominated by $\| \lceil H \rfloor_s^{-1} \|_2$. (In § 3, we show that almost diagonality of $\tilde{U}^* H \tilde{U}$ implies almost diagonality of $\lceil \tilde{U}^* H \tilde{U} \rfloor$.) However, if the matrix H is too ill–conditioned for the fast diagonalization method used to compute $\tilde{U}$, the matrices $\tilde{U}^* H \tilde{U}$ and $\tilde{U}^* \lceil H \rfloor \tilde{U}$ might be badly scaled ($\| \lceil \tilde{U}^* H \tilde{U} \rfloor_s^{-1} \|_2 \gg \| \lceil H \rfloor_s^{-1} \|_2$, $\| (\tilde{U}^* \lceil H \rfloor \tilde{U})_s^{-1} \|_2 \gg \| \lceil H \rfloor_s^{-1} \|_2$) and the estimates in Theorem 2.1 and Theorem 2.2 might be useless.

It is clear from Theorem 2.1 that there are other possibilities than spectral decomposition of H to compute the matrix $\tilde{U}$. In Theorem 2.1, the quality of $\tilde{U}$ as preconditioner is measured by its diagonalizing effect on $\lceil H \rfloor$ rather that H itself. Since $\lceil H \rfloor$ is positive definite, spectral decomposition of $\lceil H \rfloor$ is numerically more feasible than the spectral decomposition of H. However, this is not practical since $\lceil H \rfloor$ is hard to compute. The next choice is feasible from both the theoretical and the practical point of view: the SVD of H. If $H = U \Lambda U^*$, $H = W \Sigma V^*$ are the spectral and the singular value decomposition of H, respectively, then we can write $\Sigma = |\Lambda|$ and $\lceil H \rfloor = W \Sigma W^* = V \Sigma V^*$. This means that we can use computed matrices $\tilde{W} \approx W$ or $\tilde{V} \approx V$ as preconditioners. This might be better choice if H is such that fast methods such as the QR or the divide and conquer method are better as SVD than as eigenvalue solvers.

A caveat is in order here: The SVD glues together the eigenvalues of H with equal moduli and opposite signs. Consequently, the corresponding spectral subspaces (direct sums of the eigenspaces corresponding to the eigenvalues glued into a single singular value) are seen in the SVD as single singular subspaces and the preconditioned matrix is not necessarily diagonally dominant. To be more precise, let us write Λ as $\Lambda = \oplus_i \Lambda^{(i)}$, where each $\Lambda^{(i)}$ is either of the form $\lambda^{(i)} I_{p_i}$ ($\lambda^{(i)}$ is an eigenvalue of H with multiplicity p_i and $-\lambda^{(i)}$ is not in the spectrum of H) or of the form $\lambda^{(i)} I_{p_i} \oplus (-\lambda^{(i)} I_{n_i})$ ($\lambda^{(i)} > 0$ is an eigenvalue of H with multiplicity p_i and $-\lambda^{(i)}$ is an eigenvalue with multiplicity n_i). In that case we can write

$$\Sigma = |\Lambda| = J\Lambda = \oplus_i |\Lambda^{(i)}| = \oplus_i \sigma_i I_{s_i},$$

where each s_i is p_i or $p_i + n_i$, and $J = \mathrm{diag}(\mathrm{sign}(\Lambda_{ii}))$. One matrix form of the SVD of H is then $H = (UJ)|\Lambda|U^*$. If $H = W\Sigma V^*$ is another matrix SVD of H, then $V = U(\oplus_i Q_i)$ where each Q_i is some unitary matrix of order s_i. Hence, the matrix V^*HV is block–diagonal,

$$V^*HV = \oplus_i Q_i^* \Lambda^{(i)} Q_i,$$

where each $Q_i^*\Lambda^{(i)}Q_i$ is either $\lambda^{(i)} I_{p_i}$ or $\lambda^{(i)} Q_i^*(I_{p_i} \oplus (-I_{n_i}))Q_i$. If $V = [V_1, \ldots]$ is the corresponding column block–partition of V, then $Q_i^*\Lambda^{(i)}Q_i = V_i^*HV_i$ is the restriction of H to $\mathrm{span}(V_i)$. In the extreme case, $|\Lambda|$ is a scalar and the preconditioned matrix is generally dense. Important thing to note is that the diagonal blocks are scalar multiples of reflection matrices, thus with spectral condition numbers equal to one. Taking the spectral absolute value turns these blocks into diagonal matrices. This is in accordance with the fact that $\lvert V^*HV \rvert = V^* \lvert H \rvert V$ and that $\lvert \cdot \rvert$ does the same gluing as the SVD.

Consider now the computed approximation $\tilde{V} \approx V$. If $\tilde{V}$ is sufficiently accurate, then

$$\tilde{V}^* H \tilde{V} = (\oplus_i Q_i'^*)\, U'^* H U\, (\oplus_i Q_i')\,, \tag{23}$$

where Q_i' are unitary, U' is almost unitary, and U'^*HU is s.d.d. More precisely, there are scalar matrices D_i such that

$$\tilde{V}^* H \tilde{V} = (\oplus_i Q_i'^* D_i)\,(\oplus_i J_i + N)\,(\oplus_i D_i Q_i') = \oplus_i D_i\,(\oplus_i Q_i'^* J_i Q_i' + (\oplus_i Q_i'^*) N (\oplus_i Q_i'))\oplus_i D_i, \tag{24}$$

where $J_i = \mathrm{diag}(\pm 1)$, $\|N\|_2 < 1$. In other words, $\tilde{V}$ nearly decouples the eigenvalues of $\lvert H \rvert$ (or the singular values of H) and the signs of the eigenvalues with the same magnitude are determined by analyzing the diagonal blocks. In the practice, we can use the multiplicities (or clustering) of the computed singular values to forecast the block structure of the computed matrix $\tilde{V}^*H\tilde{V}$. Whether a multiple singular value (or a cluster of singular values) is a result of a genuine multiple eigenvalue (cluster of relatively close eigenvalues) or is a result of gluing of eigenvalues with opposite signs is determined after preconditioning. We finally note that we can write the matrix $\tilde{V}^*H\tilde{V}$ in relation (24) as $D(E+N')D$ where $E = E^* = E^{-1}$ and $ED = DE$. Such matrices are known to be well behaved and they include the class of s.d.d. matrices (cf. [25, Theorem 2.29]). Theorem 3.1 below describes the absolute value of such matrices.

In the next two examples, we show that preconditioning using approximate eigenvector matrix $\tilde{U}$, computed by fast diagonalization methods such as the divide and conquer or the QR method, might spoil the accuracy of the eigenvalues of the matrix. On the other hand, using approximate singular vectors of H, computed by the SVD versions of these methods, yields good accuracy.

Example 2.1 We generate an 8×8 double precision indefinite matrix H with $\kappa_2(H) \approx 1.353\cdot 10^{17}$, $\|H\|_2 \approx 0.5 \cdot 10^8$, $\kappa_2(\lvert H \rvert_s) \approx 69.775$. Hence, the eigenvalues less that 10^{-8} (roughly) in modulus cannot be approximated accurately by methods based on tridiagonalization, even in the double precision computation (round–off $\approx 10^{-16}$). On the other hand, a variant of the Jacobi method that uses the symmetric indefinite decomposition $\Pi^\tau H \Pi = GJG^\tau$ and then implicitly diagonalizes the pencil $G^\tau G - \lambda J$ (cf. [24], [22]) in this case approximates all eigenvalues with guaranteed high relative accuracy, even in single precision computation (round–off $\approx 10^{-8}$). We use double precision implementation of this procedure to compute the reference values $\tilde{\lambda}_{1,D} \geq \cdots \geq \tilde{\lambda}_{8,D}$. We use two different preconditioning matrices: the matrix $\tilde{U}$ computed using the symmetric eigenvalue solver `SSYEVD()` and the matrix $\tilde{Q}$ computed as the left singular vector matrix of H, using `SGESVD()` (from LAPACK). The corresponding preconditioned matrices are denoted by $H' = \tilde{U}^\tau H \tilde{U}$, $H'' = \tilde{Q}^\tau H \tilde{Q}$. The eigenvalues computed by application of the symmetric Jacobi method to H' and H'' are denoted by $\tilde{\lambda}_1' \geq \cdots \geq \tilde{\lambda}_8'$ and $\tilde{\lambda}_1'' \geq \cdots \geq \tilde{\lambda}_8''$, respectively. We use $(\tilde{\lambda}_{i,D})$ to compute the relative errors

$$\epsilon_i' = \frac{|\tilde{\lambda}_i' - \tilde{\lambda}_{i,D}|}{|\tilde{\lambda}_{i,D}|}, \quad \epsilon_i'' = \frac{|\tilde{\lambda}_i'' - \tilde{\lambda}_{i,D}|}{|\tilde{\lambda}_{i,D}|}, \quad 1 \leq i \leq 8.$$

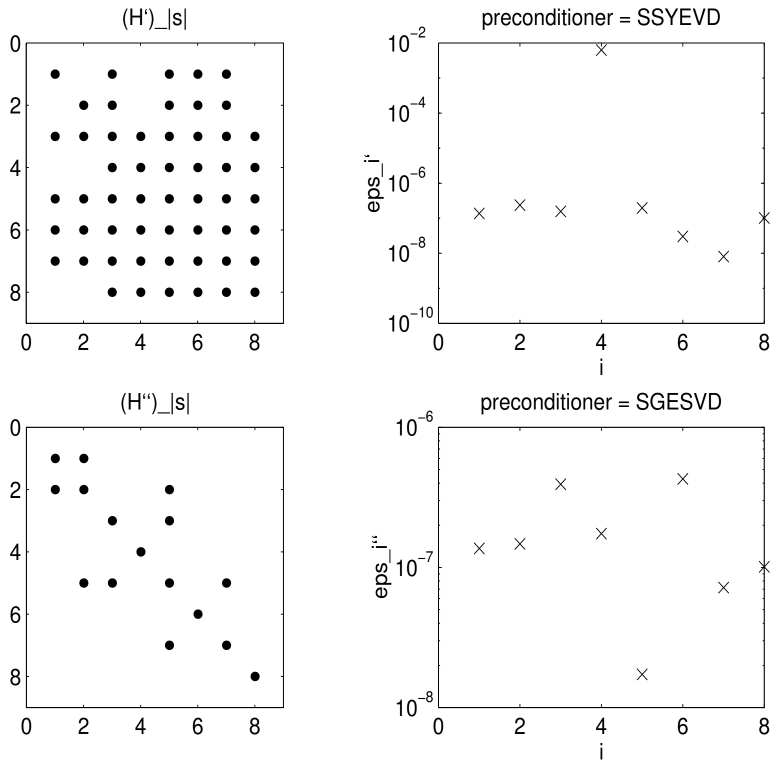

Figure 1: The scaled diagonal dominance and relative accuracy of the computed eigenvalues on the 8×8 indefinite matrix from Example 2.1. The approximate eigenvectors are computed using using the LAPACK's procedures `SSYEVD()` and `SGESVD()`.

To measure the effect of preconditioning, we compute the matrices

$$H'_{|s|} = \mathrm{diag}(|H'|_{ii})^{-1/2} H' \mathrm{diag}(|H'|_{ii})^{-1/2}, \quad H''_{|s|} = \mathrm{diag}(|H''|_{ii})^{-1/2} H'' \mathrm{diag}(|H''|_{ii})^{-1/2},$$

and set to zero those elements of $H'_{|s|}$ and $H''_{|s|}$ which are below some given tolerance `tol`. Then we use MATLAB's `spy()` function to investigate the structure of $H'_{|s|}$ and $H''_{|s|}$. The results are displayed in Figure 1, where we use $\mathtt{tol} = 10^{-4}$.

The relative error of order 10^{-2} in $\tilde{\lambda}'_4$ is caused by surprisingly high $\kappa_2(\lvert H' \rvert_s)$ ($\kappa_2(\lvert H' \rvert_s) \approx 2.156 \cdot 10^6$). We also note that maximal off–diagonal element of $H'_{|s|}$ is about 1.5725. (Similar results are obtained using `SSYEV()` instead of `SSYEVD()`.) On the other hand, the results obtained by using $\tilde{Q}$ (second row in Figure 1) are much better. More precisely, $\kappa_2(\lvert H'' \rvert_s) \approx 1.023$, the maximal off–diagonal element of $H''_{|s|}$ is about $1.121 \cdot 10^{-2}$, and $\max_{1 \le i \le 8} \epsilon''_i < 4.3 \cdot 10^{-7}$.

Example 2.2 Our next example is a 5×5 indefinite matrix H with $\kappa_2(H) \approx 1.41 \cdot 10^{40}$ and $\kappa_2(\lvert H \rvert_s) \approx 53.53$. We use the same strategy and the same notation as in the previous example. To emphasize the difference between $H'_{|s|}$ and $H''_{|s|}$, we set an element of $H'_{|s|}$ to zero if it is less than 10^{-3} in modulus and an element of $H''_{|s|}$ is set to zero only if it is less than 10^{-6} in modulus. The results are shown in Figure 2. It is important to mention that $\kappa_2(\lvert H' \rvert_s) \approx 9.94 \cdot 10^7$ and that the largest off–diagonal element of $H'_{|s|}$ is between 3.2 and 3.21.

In some cases, it is possible to improve the accuracy of a fast method by its repeated use on certain submatrices of the preconditioned matrix. We will first illustrate this using a small dimension example.

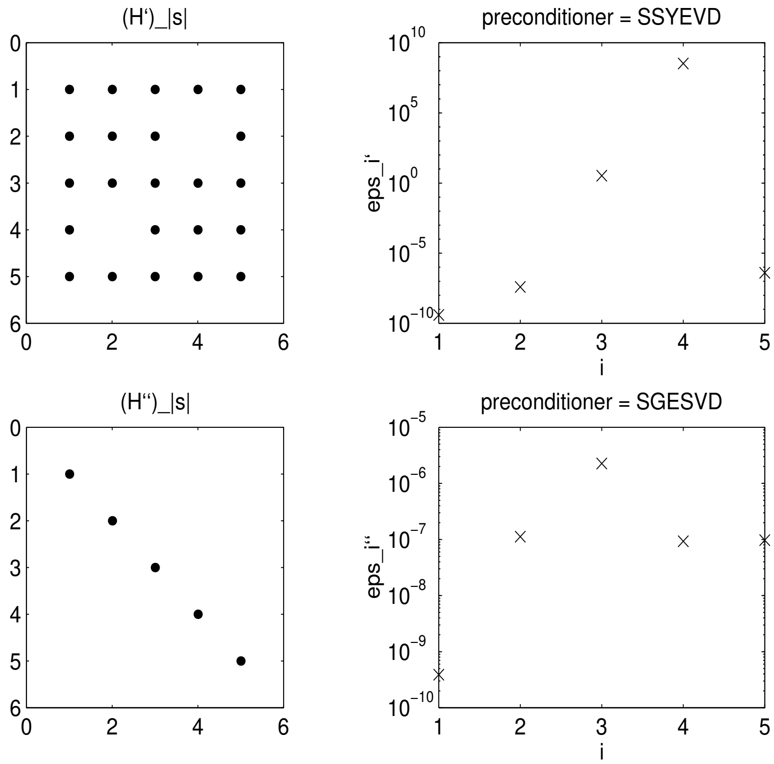

Figure 2: The scaled diagonal dominance and relative accuracy of the computed eigenvalues on the 5×5 matrix from Example 2.2. Note that the singular vectors computed by `SGESVD()` are good preconditioner, while the eigenvectors computed by `SSYEVD()` perform poorly.

Example 2.3 We generate positive definite $H = \Delta_H H_s \Delta_H$ with $\kappa_2(H_s) \approx 400$, $\kappa_2(\Delta_H) \approx 4 \cdot 10^{10}$. Then we compute the spectral decomposition of H using the procedure `SSYEVD()` from the LAPACK [1] library. (In this procedure, the spectral decomposition is computed using fast divide and conquer algorithm.) As reference values for the eigenvalues of H we use the double precision values $\tilde{\lambda}_{1,D} \leq \cdots \leq \tilde{\lambda}_{n,D}$, computed using `DSYEVD()`. For simplicity, we take small dimension example, $n = 22$. We compute the matrix $\tilde{H}'$ using BLAS 3 [4] procedures `SSYMM()` and `SGEMM()`. Here we first reorder the eigenvectors computed by `SSYEVD()` in order to have the diagonals of $\tilde{H}'$ in (approximately) nonincreasing order. In the computed scaled matrix $(\tilde{H}')_s$ we set to zero entries which are below $1.6 \cdot 10^{-6}$ in modulus. In this way, we can use the MATLAB function `spy()` to analyze the structure of the matrix. In the first picture in Figure 3, we display `spy(`$(\tilde{H}')_s$`)`. The maximal off–diagonal entry of $(\tilde{H}')_s$ is below 0.35. The relative errors in eigenvalues $\tilde{\lambda}_1 \leq \cdots \leq \tilde{\lambda}_n$ computed by `SSYEVD()` are defined as

$$\epsilon_i = \frac{|\tilde{\lambda}_{i,D} - \tilde{\lambda}_i|}{\tilde{\lambda}_{i,D}}, \quad 1 \leq i \leq n,$$

and are shown by crosses (`x`) in the second picture. It is interesting to mention that $\tilde{\lambda}_1 \approx -0.13239383 \cdot 10^{-9}$, while $\tilde{\lambda}_{1,D} \approx 0.19203695 \cdot 10^{-11}$. In the same picture, the pluses (`+`) denote the relative errors in the eigenvalues computed by an application of the symmetric Jacobi method to the computed matrix $\tilde{H}'$. Next, we write the matrix $\tilde{H}'$ as

$$\tilde{H}' = \begin{bmatrix} A' & B' \\ B'^{\tau} & K' \end{bmatrix}, \quad K' \in \mathbf{R}^{11\times 11},$$

and apply `SSYEVD()` to K' to compute approximately $K' \approx \tilde{W}\mathrm{diag}(\tilde{\lambda}_i^{(K')})\tilde{W}^{\tau}$. Then we compute $\tilde{H}'' = (I \oplus \tilde{W}^{\tau})\tilde{H}'(I \oplus \tilde{W})$ and $(\tilde{H}'')_s$ in the same way as $(\tilde{H}')_s$. The structure of $(\tilde{H}'')_s$ is shown in the third picture in Figure 3. The maximal off–diagonal entry of $(\tilde{H}'')_s$ is below 0.006. Finally, we replace the lowest 11 eigenvalues $\tilde{\lambda}_i$ with $\tilde{\lambda}_i^{(K')}$. The relative errors in the approximate spectrum is shown by crosses in the last picture. The pluses denote the relative errors from an application of the Jacobi method to $\tilde{H}''$.

The results illustrated in Example 2.3 deserve closer look. Let H and $\tilde{H}'$ be positive definite. Let

$$\tilde{H}' = \begin{bmatrix} A' & B' \\ B'^{*} & K' \end{bmatrix}, \quad (\tilde{H}')_s = \begin{bmatrix} (A')_s & (B')_s \\ ((B')_s)^* & (K')_s \end{bmatrix}, \quad A' \in \mathbf{C}^{m\times m}, \tag{25}$$

where the block partition is determined so that A' corresponds to a group of the largest m eigenvalues of $\tilde{H}'$ and K' corresponds to the remaining (smallest) eigenvalues. (This partition will be obvious if, for instance, there is a strong dichotomy in the spectrum of H.) Due to the Cauchy interlacing theorem, the spectral condition numbers of K' and A' cannot exceed the spectral condition number of $\tilde{H}'$. In fact, it is possible that $\kappa_2(A') \ll \kappa_2(\tilde{H}')$, $\kappa_2(K') \ll \kappa_2(\tilde{H}')$. Further, let $A' = L_{A'}^* L_{A'}$, where $L_{A'}$ is the Cholesky factor of A' or, for example, $L_{A'} = \sqrt{A'}$. Similarly, let $K' = L_{K'}^* L_{K'}$. Consider the factorization:

$$\tilde{H}' = \begin{bmatrix} L_{A'}^* & 0 \\ 0 & L_{K'}^* \end{bmatrix} \begin{bmatrix} I & Y \\ Y^* & I \end{bmatrix} \begin{bmatrix} L_{A'} & 0 \\ 0 & L_{K'} \end{bmatrix}, \quad Y = L_{A'}^{-*} B' L_{K'}^{-1}. \tag{26}$$

Due to positive definiteness, $\|Y\|_2 < 1$ and $\tilde{H}'$ is similar to the matrix

$$\tilde{H}'_{\sim} = \begin{bmatrix} I & Y \\ 0 & \sqrt{I - Y^*Y} \end{bmatrix} \begin{bmatrix} L_{A'}L_{A'}^* & 0 \\ 0 & L_{K'}L_{K'}^* \end{bmatrix} \begin{bmatrix} I & 0 \\ Y^* & \sqrt{I - Y^*Y} \end{bmatrix}. \tag{27}$$

Here we use the factorization

$$\begin{bmatrix} I & Y \\ Y^* & I \end{bmatrix} = \begin{bmatrix} I & 0 \\ Y^* & \sqrt{I - Y^*Y} \end{bmatrix} \begin{bmatrix} I & Y \\ 0 & \sqrt{I - Y^*Y} \end{bmatrix} \equiv \mathcal{Y}\mathcal{Y}^*$$

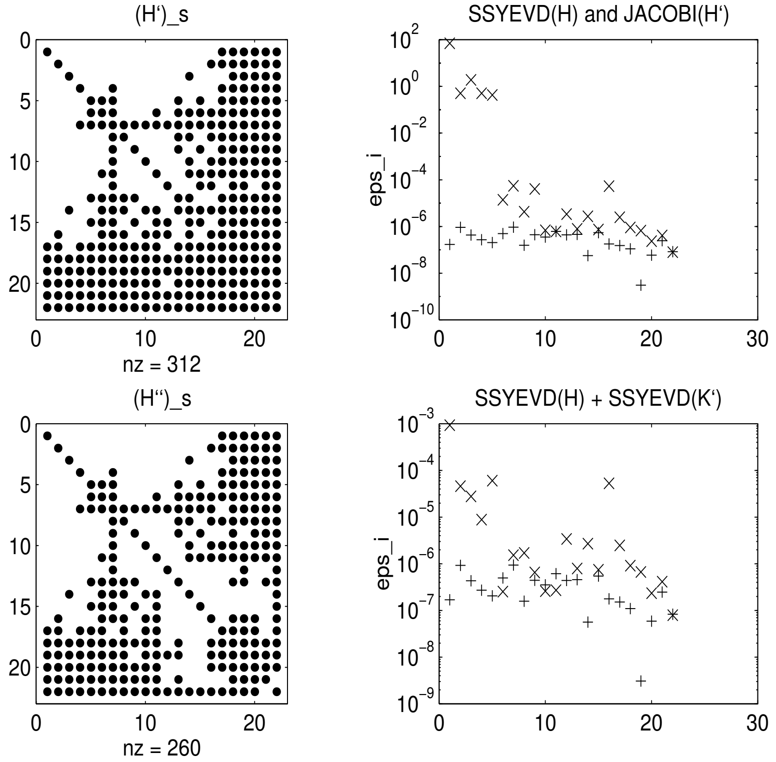

Figure 3: An illustration of improved accuracy using `SSYEVD()` on a submatrix of the preconditioned matrix from Example 2.3.

and the fact that the matrices AB and $BA = B(AB)B^{-1}$ are similar. Hence, if $\tilde{\lambda}'_1 \geq \cdots \geq \tilde{\lambda}'_n$ are the eigenvalues of $\tilde{H}'$ and if $\lambda_{1,\bowtie} \geq \cdots \geq \lambda_{n,\bowtie}$ are the ordered values of the union of the spectra of A' and K', then there exist real numbers $\theta_1, \ldots, \theta_n$ such that

$$\tilde{\lambda}'_i = \theta_i \lambda_{i,\bowtie}, \quad 1 - \|Y\|_2 \leq \theta_i \leq 1 + \|Y\|_2. \tag{28}$$

This estimate can be improved as follows. From an estimate of Li [17], it follows that

$$\max_{1\leq i\leq n} \frac{|\tilde{\lambda}'_i - \lambda_{i,\bowtie}|}{\sqrt{\tilde{\lambda}'_i \lambda_{i,\bowtie}}} \leq \|\mathcal{Y}^* - \mathcal{Y}^{-1}\|_2. \tag{29}$$

An elementary calculation shows that

$$\mathcal{Y}^* - \mathcal{Y}^{-1} = \begin{bmatrix} I & 0 \\ 0 & (I - Y^\tau Y)^{-1/2} \end{bmatrix} \begin{bmatrix} 0 & Y \\ Y^\tau & -Y^\tau Y \end{bmatrix} \tag{30}$$

and using the SVD of Y we easily compute

$$\|\mathcal{Y}^* - \mathcal{Y}^{-1}\|_2 = \frac{\|Y\|_2}{\sqrt{1 - \|Y\|_2}}. \tag{31}$$

Note that generally holds $\|Y\|_2 \leq \sqrt{\|(A')_s^{-1}\|_2 \|(K')_s^{-1}\|_2} \|(B')_s\|_2$. In Example 2.3 we obtain, using MATLAB, that $\|Y\|_2 \approx 8.09 \cdot 10^{-3}$, $\|(B')_s\|_2 \approx 7.47 \cdot 10^{-3}$, $\kappa_2(K') \approx 2.6 \cdot 10^4$, and $\sqrt{\|(A')_s^{-1}\|_2 \|(K')_s^{-1}\|_2} \|(B')_s\|_2 \approx 1.04 \cdot 10^{-2}$. Hence, the improved relative accuracy of order 10^{-3} at the left end of the spectrum is in accordance with the theory. We can obviously apply the same strategy to A' and K' and solve a sequence of smaller problems to finally diagonalize A' and K'. If the eigenvalues of H are relatively well separated then the relative error bound is quadratic in $\|Y\|_2$. More precisely, we have the following lemma (cf. [8]).

Lemma 2.1 *Let in relation (25) the matrix $\tilde{H}'$ be positive definite and let the matrices A' and K' be diagonal. Let λ be an eigenvalue of $\tilde{H}'$ and let $A' = \Gamma_\lambda \oplus \hat{\Gamma}_\lambda$, $K' = \Xi_\lambda \oplus \hat{\Xi}_\lambda$ be such partitions that*

$$\|\lambda\Gamma_\lambda^{-1} - I\|_2 \leq \|Y\|_2, \quad \|\lambda\Xi_\lambda^{-1} - I\|_2 \leq \|Y\|_2$$

and such that for some $\alpha > \|Y\|_2$ and $\beta > \|Y\|_2$

$$\sigma_{\min}(\lambda\hat{\Gamma}_\lambda^{-1} - I) \geq \alpha, \quad \sigma_{\min}(\lambda\hat{\Xi}_\lambda^{-1} - I) \geq \beta.$$

(Here $\sigma_{\min}(\cdot)$ denotes the minimal singular value of a matrix.) In other words, Γ_λ and Ξ_λ contain those values of $(\lambda_{i,\bowtie})_{i=1}^n$ which approximate λ in the sense of relation (29), and $\hat{\Gamma}_\lambda$, $\hat{\Xi}_\lambda$ contain the remaining values of $(\lambda_{i,\bowtie})_{i=1}^n$. The values of α and β give the relative separation between λ and the non–matching eigenvalues from the spectrum of $A' \oplus K'$. If $\Gamma_\lambda \oplus \Xi_\lambda$ is of the order of the multiplicity of λ, then it holds for any unitarily invariant norm $\|\cdot\|$ that

$$\|I - \lambda\Gamma_\lambda^{-1}\| \leq \frac{1}{1-\gamma} \frac{\|Y\|_2 \|Y\|}{\beta}, \tag{32}$$

$$\|I - \lambda\Xi_\lambda^{-1}\| \leq \frac{1}{1-\gamma} \frac{\|Y\|_2 \|Y\|}{\alpha}, \tag{33}$$

where $\gamma = \|Y\|_2^2/(\alpha\beta)$.

The case of indefinite matrix $\tilde{H}'$ is less simple. We first write A' and K' from (25) as $A' = L_{A'}^* J_{A'} L_{A'}$, $K' = L_{K'}^* J_{K'} L_{K'}$, where $J_{A'}$ and $J_{K'}$ are the inertia matrices (diagonal with diagonal entries ± 1). Such decompositions always exist. Next, we replace the factorization (26) with

$$\tilde{H}' = \begin{bmatrix} L_{A'}^* & 0 \\ 0 & L_{K'}^* \end{bmatrix} \begin{bmatrix} J_{A'} & Y \\ Y^* & J_{K'} \end{bmatrix} \begin{bmatrix} L_{A'} & 0 \\ 0 & L_{K'} \end{bmatrix} \equiv G\tilde{J}G^*, \quad Y = L_{A'}^{-*} B' L_{K'}^{-1},$$

and we note that the eigenvalues of $\tilde{H}'$ are also the eigenvalues of the definite matrix pencil $\tilde{J}-\lambda M$, $M=(G^*G)^{-1}$. Now, consider $\tilde{J}-\lambda M$ as perturbation of the pencil $J-\lambda M$, where $J=J_{A'}\oplus J_{K'}$. Obviously, the eigenvalues $\lambda_{1,\bowtie}\geq\cdots\geq\lambda_{n,\bowtie}$ of $J-\lambda M$ are the union of the eigenvalues of A' and K'. Using [25, Theorem 2.1] we conclude that

$$1-\eta\leq\frac{\tilde{\lambda}'_i}{\lambda_{i,\bowtie}}\leq 1+\eta, \tag{34}$$

where

$$\eta\equiv\max_{x\neq 0}\frac{|x^*\delta Jx|}{x^*|J|_M x},\quad \delta J=\tilde{J}-J, \tag{35}$$

and provided that $\eta<1$. Here $|J|_M$ is defined as follows: For any factorization $M=ZZ^*$,

$$|J|_M=Z|Z^{-1}JZ^{-*}|Z^*.$$

Note that

$$|J|_M=\begin{bmatrix}|J_{A'}|_{L_{A'}^{-*}L_{A'}^{-1}} & 0\\ 0 & |J_{K'}|_{L_{K'}^{-*}L_{K'}^{-1}}\end{bmatrix},\quad \delta J=\begin{bmatrix}0 & L_{A'}^{-*}B'L_{K'}^{-1}\\ L_{K'}^{-*}(B')^*L_{A'}^{-1} & 0\end{bmatrix}.$$

Further, if $L_{A'}^*J_{A'}L_{A'}=W\Lambda_{A'}W^*$, $L_{K'}^*J_{K'}L_{K'}=V\Lambda_{K'}V^*$ are the spectral decompositions of A', K', then (cf. [25])

$$\begin{aligned}|J_{A'}|_{L_{A'}^{-*}L_{A'}^{-1}} &= \left(L_{A'}^{-*}W|\Lambda_{A'}|^{1/2}\right)\left(L_{A'}^{-*}W|\Lambda_{A'}|^{1/2}\right)^*,\\ |J_{K'}|_{L_{K'}^{-*}L_{K'}^{-1}} &= \left(L_{K'}^{-*}V|\Lambda_{K'}|^{1/2}\right)\left(L_{K'}^{-*}V|\Lambda_{K'}|^{1/2}\right)^*.\end{aligned}$$

Hence, $|J|_M=\mathcal{M}\mathcal{M}^*$, where $\mathcal{M}=\left(L_{A'}^{-*}W|\Lambda_{A'}|^{1/2}\right)\oplus\left(L_{K'}^{-*}V|\Lambda_{K'}|^{1/2}\right)$. From this, it follows that

$$\begin{aligned}\eta &= \max_{x^*x=1}|x^*(\mathcal{M}^{-1}\delta J\mathcal{M}^{-*})x|,\\ \mathcal{M}^{-1}\delta J\mathcal{M}^{-*} &= \begin{bmatrix}0 & |\Lambda_{A'}|^{-1/2}W^*B'V|\Lambda_{K'}|^{-1/2}\\ |\Lambda_{K'}|^{-1/2}V^*(B')^*W|\Lambda_{A'}|^{-1/2} & 0\end{bmatrix}.\end{aligned}$$

Thus,

$$\eta=\||A'|^{-1/2}B'|K'|^{-1/2}\|_2. \tag{36}$$

If A' and K' are definite and if $L_{A'}$ and $L_{K'}$ are the Cholesky factors, then for any unitarily invariant norm $\eta=\|Y\|$. If A' and K' are diagonal, then $\eta=\||\Lambda_{A'}|^{-1/2}B'|\Lambda_{K'}|^{-1/2}\|_2$. Next, we note that an estimate quadratic in η (similar as in the definite case) can be derived using the results from [10]. More precisely, we have the following lemma.

Lemma 2.2 *Let A' and K' be diagonal with eigenvalues $\lambda_{1,\bowtie}\geq\cdots\geq\lambda_{m,\bowtie}$ and $\lambda_{m+1,\bowtie}\geq\cdots\geq\lambda_{n,\bowtie}$, respectively. Further, let $\lambda_{m,\bowtie}>\lambda_{m+1,\bowtie}$ and let*

$$\gamma=\min_{\tilde{\lambda}'_i\neq\tilde{\lambda}'_j}\frac{|\tilde{\lambda}'_i-\tilde{\lambda}'_j|}{|\tilde{\lambda}'_i|+|\tilde{\lambda}'_j|}.$$

If

$$\eta_F\equiv\|\,|A'|^{-1/2}B'|K'|^{-1/2}\|_F<\frac{\gamma}{\gamma+3},$$

then

$$\sqrt{\sum_{i=1}^{n}\left(\frac{\lambda_{i,\bowtie}-\tilde{\lambda}'_i}{\lambda_{i,\bowtie}}\right)^2}\leq\frac{\sqrt{8}}{\gamma}\eta_F^2. \tag{37}$$

The preceding discussion naturally leads to the problem of approximation of a part of the spectrum of H from suitably chosen m–dimensional subspace with $m \ll n$. More precisely, if $\tilde{U}_\partial$ is $n \times m$ nearly orthonormal matrix of approximate eigenvectors of H (more generally, $\tilde{U}_\partial$ spans an approximate invariant subspace of H), what can we say about the distance between the eigenvalues of the computed (inexact) Rayleigh matrix $\tilde{H}'_\partial = \tilde{U}^*_\partial H \tilde{U}_\partial + \delta H'_\partial$ and the spectrum of H? To answer this question, we can first embed $\tilde{U}_\partial$ into a nearly orthogonal matrix $\tilde{U}$ as $\tilde{U} = [\tilde{U}_\partial, \tilde{U}_\partial^\perp]$, where $\tilde{U}_\partial^\perp$ is exactly orthonormal basis for the (exact) orthogonal complement of $\mathcal{U} = \mathrm{span}(\tilde{U})$. Then we can use Theorems 2.1 and 2.2 and relations (25–37) to compare the eigenvalues of $\tilde{H}'_\partial$ with part of the spectrum of $\tilde{H}'$. However, these estimates use information from the orthogonal complement of $\mathcal{U}$ and, therefore, are not easily computable in practice. Another approach, based on the results from [6], uses $H, \mathcal{U}$ and H^{-1}.

Lemma 2.3 *Let $\tilde{\lambda}_{1,\partial} \geq \cdots \geq \tilde{\lambda}_{m,\partial}$ be the eigenvalues of $\tilde{H}'_\partial$. Let $\mathcal{V} = H\mathcal{U}$, $\mathcal{W} = H^{-1}\mathcal{U}$, and let $\phi = \angle(\mathcal{U}, \mathcal{V})$, $\psi = \angle(\mathcal{V}, \mathcal{W})$, where the angle $\angle$ is defined as the maximal principal angle between two subspaces. Then there exist m eigenvalues $\lambda_{i_1} \geq \cdots \geq \lambda_{i_m}$ of $\tilde{H}'$ and there exist $\epsilon_1, \ldots, \epsilon_m$ such that*

$$\tilde{\lambda}_{i,\partial} = \tilde{\lambda}'_i(1+\epsilon_i), \quad |\epsilon_i| \leq \sin\phi + \tan\psi, \quad i = 1, \ldots, m. \tag{38}$$

The overall error bound can be improved if we use the fact that the rounding errors compose a perturbation of rank at most m. A consequence of this fact is that in Theorems 2.1 and 2.2 the eigenvalues of $\tilde{H}'$ are better approximations of the eigenvalues of H. For instance, one can show that in Theorem 2.2 the matrix $|\tilde{H}'|$ can be replaced with $|\tilde{H}'_\partial|$.

3 On the spectral absolute value of a s.d.d. H

Note that both Theorem 2.1 and Theorem 2.2 make use of the pretransformed spectral absolute value $\tilde{U}^*|H|\tilde{U}$. On one hand this is natural, because it is just $|H|$ which appears in the perturbation theorem Theorem 1.1. On the other hand, it is not $\tilde{U}^*|H|\tilde{U}$ which appears in our computations but $\tilde{U}^*H\tilde{U}$. While we can check whether the latter came out scaled diagonally dominant, this is not easy to do for the former. Since the eigenvectors of H are also the eigenvectors of $|H|$ the latter matrix is expected to be at least about as diagonal as the former, just think of H which is, in addition, unitary, in which case $|H|$ is simply a scalar. The two-by-two case is also very instructive. Using Lagrange interpolation polynomial we find

$$|H| = \frac{|\lambda_1| - |\lambda_2|}{\lambda_1 - \lambda_2} H - \frac{\lambda_2|\lambda_1| - |\lambda_2|\lambda_1}{\lambda_1 - \lambda_2} I$$

and we see that the impact of H is "dumped" with the factor $||\lambda_1| - |\lambda_2||/|\lambda_1 - \lambda_2| \leq 1$. Numerical experiments on "random" s.d.d. matrices show the same phenomenon: taking the spectral absolute value causes very small loss of scaled diagonal dominance.

In this section we give rigorous estimates of this type. They may have independent interest. For generality, we consider the matrices of the form $H = D(E+N)D$, where D is diagonal, $E = E^* = E^{-1}$ commutes with D and $\|N\|_2$ is small. Such matrices may be called *block s.d.d. matrices*. They are an immediate generalization of the common s.d.d. matrices and have similar properties ([25]).

Lemma 3.1 *Let $H = D(E+N)D$ be a Hermitian matrix with $E = E^* = E^{-1}$, diagonal nonsingular matrix D such that $ED = DE$ and $\|N\|_2 \leq \gamma < 1/2$. Let $|H| = DAD$ and $H^{-1} = D^{-1}(E+N_1)D^{-1}$. Then $\|N_1\|_2 \leq \|N\|_2/(1 - \|N\|_2)$ and*

$$\mathrm{Trace}(A) \leq \frac{n}{1 - \|N_1\|_2}, \tag{39}$$

$$\mathrm{Trace}(A^{-1}) \leq \frac{n}{1 - \|N\|_2}. \tag{40}$$

Proof Let $H = U\Lambda U^*$ be the spectral decomposition of H. Then

$$A = D^{-1}U|\Lambda|U^*D^{-1}, \quad A^{-1} = DU|\Lambda|^{-1}U^*D.$$

Using [25, Theorem 2.29], we have

$$\frac{1}{1+\|N\|_2} \le \|DUe_i|\lambda_i|^{-1/2}\|_2^2 \le \frac{1}{1-\|N\|_2}, \tag{41}$$

and, since $\mathrm{Trace}(A^{-1}) = \mathrm{Trace}(|\Lambda|^{-1/2}U^*D^2U|\Lambda|^{-1/2})$, we can easily establish (40). Next, note that the matrix $H^{-1} = D^{-1}(E+N)^{-1}D^{-1}$ is s.d.d. as well, because

$$(E+N)^{-1} = E\sum_{k=0}^{\infty}(-1)^k(NE)^k = E + N_1, \;\; \|N_1\|_2 \le \frac{\|N\|_2}{1-\|N\|_2} < 1.$$

Hence, relation (40) implies (39). Q.E.D.

Corollary 3.1 *Let the assumptions of Lemma 3.1 hold and let*

$$\gamma = \max\{\|N\|_2, \|N_1\|_2\}, \quad \eta = \frac{2n\gamma}{1-\gamma}.$$

Then

$$\max\{\|A-I\|_2, \|A^{-1}-I\|_2\} \le \frac{n\gamma + \sqrt{n\gamma}\sqrt{2+(n-2)\gamma}}{1-\gamma}. \tag{42}$$

Proof From relations (39) and (40), it follows that the eigenvalues $\alpha_1 \ge \cdots \ge \alpha_n$ of A satisfy

$$\alpha_i + \frac{1}{\alpha_i} \le 2 + 2\eta, \quad 1 \le i \le n. \tag{43}$$

Indeed, we can write, for all i,

$$\alpha_i + \frac{1}{\alpha_i} \le \frac{2n}{1-\gamma} - \sum_{j\ne i}(\alpha_j + \frac{1}{\alpha_j}),$$

and use the fact that $\alpha_j + 1/\alpha_j \ge 2$. Hence, for all i,

$$1 + \frac{\eta}{2} - \sqrt{\eta + \frac{\eta^2}{4}} \le \frac{1}{\alpha_i},\ \alpha_i \le 1 + \frac{\eta}{2} + \sqrt{\eta + \frac{\eta^2}{4}}, \tag{44}$$

and (42) follows. Q.E.D.

Thus, for sufficiently small $\|N\|_2$, the matrix $|H|$ is s.d.d. as well. Note, however, that for $\gamma \to 0$, the estimate (42) is dominated by $\sqrt{2n\gamma}$.

Theorem 3.1 *Let $H = D(E+N)D$ be as in Lemma 3.1. Further, let $H(\varepsilon) = D(E+\varepsilon N)D$, $0 \le \varepsilon \le 1$, and let $A(\varepsilon) = D^{-1}|H(\varepsilon)|D^{-1}$. Then $|H|$ can be factored as $|H| = D(I+M)D$, where*

$$\|M\|_F \le \|N\|_F \int_0^1 \kappa_2(A(\varepsilon))d\varepsilon, \tag{45}$$

$$\int_0^1 \kappa_2(A(\varepsilon))d\varepsilon \le 1 + \frac{2n\|N\|_2}{1-2\|N\|_2} + \frac{2(n\|N\|_2)^2}{1-2\|N\|_2} + \frac{4}{3}\frac{(1+n\|N\|_2)^{3/2}}{(1-2\|N\|_2)^2}\sqrt{n\|N\|_2}. \tag{46}$$

Proof Consider the Hermitian analytic matrix family

$$H(\varepsilon) = D(E + \varepsilon N)D, \quad 0 \le \varepsilon \le 1, \tag{47}$$

of s.d.d. matrices. The derivative

$$Z(\varepsilon) = \frac{d}{d\varepsilon}|H(\varepsilon)|$$

satisfies the Lyapunov equation

$$|H(\varepsilon)|Z(\varepsilon) + Z(\varepsilon)|H(\varepsilon)| = H(\varepsilon)DND + DNDH(\varepsilon) \tag{48}$$

and it holds that

$$\frac{d}{d\varepsilon}A(\varepsilon) = D^{-1}\frac{d}{d\varepsilon}|H(\varepsilon)|D^{-1} = D^{-1}Z(\varepsilon)D^{-1}. \tag{49}$$

We solve the Lyapunov equation (48) by diagonalizing $H(\varepsilon)$ as

$$H(\varepsilon) = U_\varepsilon \Lambda_\varepsilon U_\varepsilon^*,\ \Lambda_\varepsilon = \mathrm{diag}\,(\lambda_{\varepsilon,1}, \ldots, \lambda_{\varepsilon,n}),\ \ U_\varepsilon \text{ unitary.}$$

Then $Z(\varepsilon) = U_\varepsilon W(\varepsilon) U_\varepsilon^*$, where $W(\varepsilon)$ is the solution of the equation

$$|\Lambda_\varepsilon|W(\varepsilon) + W(\varepsilon)|\Lambda_\varepsilon| = \Lambda_\varepsilon U_\varepsilon^* DNDU_\varepsilon + U_\varepsilon^* DNDU_\varepsilon \Lambda_\varepsilon. \tag{50}$$

This simplifies, if we take $\varepsilon = 0$. Then $W(0) = Z(0)$ and

$$D^2 Z(0) + Z(0)D^2 = D^3 END + DNED^3 \tag{51}$$

from which we obtain

$$\left(\frac{d}{d\varepsilon}A(\varepsilon)\Big|_{\varepsilon=0}\right)_{ij} = \frac{D_{ii}^2(EN)_{ij} + D_{jj}^2(NE)_{ij}}{D_{ii}^2 + D_{jj}^2}. \tag{52}$$

This provides a valuable information, but only asymptotically. To estimate $A(1) = I + M$, we need a bound for the derivative of $A(\varepsilon)$ over the whole interval $(0, 1)$. From (50), it follows that

$$\frac{d}{d\varepsilon}A(\varepsilon) = D^{-1}U_\varepsilon(\Xi_\varepsilon \circ (U_\varepsilon^* DNDU_\varepsilon))U_\varepsilon^* D^{-1}, \tag{53}$$

where $\circ$ denotes the Hadamard matrix product and

$$(\Xi_\varepsilon)_{ij} = \frac{\lambda_{\varepsilon,i} + \lambda_{\varepsilon,j}}{|\lambda_{\varepsilon,i}| + |\lambda_{\varepsilon,j}|}, \quad 1 \le i, j \le n.$$

We can write the relation (53) as

$$\frac{d}{d\varepsilon}A(\varepsilon) = D^{-1}U_\varepsilon|\Lambda_\varepsilon|^{1/2}(\Xi_\varepsilon \circ (|\Lambda_\varepsilon|^{-1/2}U_\varepsilon^* DNDU_\varepsilon|\Lambda_\varepsilon|^{-1/2}))|\Lambda_\varepsilon|^{1/2}U_\varepsilon^* D^{-1},$$

and, using the properties of the Frobenius and the spectral norms, we obtain

$$\|\frac{d}{d\varepsilon}A(\varepsilon)\|_F \le \|DU_\varepsilon|\Lambda_\varepsilon|^{-1/2}\|_2^2 \|D^{-1}U_\varepsilon|\Lambda_\varepsilon|^{1/2}\|_2^2 \|N\|_F = \kappa_2(A(\varepsilon))\|N\|_F, \tag{54}$$

and

$$\|A - I\|_F = \|\int_0^1 dA(\varepsilon)\|_F \le \|N\|_F \int_0^1 \kappa_2(A(\varepsilon))d\varepsilon. \tag{55}$$

Next we integrate $\kappa_2(A(\varepsilon))$. If $\alpha_1(\varepsilon) \ge \cdots \ge \alpha_n(\varepsilon)$ are the eigenvalues of $A(\varepsilon)$, then an estimate similar to (44) holds with η replaced by

$$\eta(\varepsilon) = \frac{2n\varepsilon\|N\|_2}{1 - 2\varepsilon\|N\|_2} \le \frac{2n\varepsilon\|N\|_2}{1 - 2\|N\|_2}.$$

Hence,

$$\kappa_2(A(\varepsilon)) \leq 1 + 2\eta(\varepsilon) + \frac{\eta(\varepsilon)^2}{2} + \bar{\eta}(\varepsilon), \quad \bar{\eta}(\varepsilon) \equiv (2+\eta(\varepsilon))\sqrt{\eta(\varepsilon)}\sqrt{1+\frac{\eta(\varepsilon)}{4}}. \tag{56}$$

An elementary calculation yields

$$\begin{aligned}
\int_0^1 \eta(\varepsilon)d\varepsilon &= n\left(-1 + \frac{|\ln(1-2\|N\|_2)|}{2\|N\|_2}\right) \leq \frac{n\|N\|_2}{1-2\|N\|_2}, \\
\int_0^1 \eta(\varepsilon)^2 d\varepsilon &= \frac{n^2}{2\|N\|_2}\int_0^{2\|N\|_2} \frac{\zeta^2}{(1-\zeta)^2}d\zeta = n^2\sum_{k=2}^{\infty}(2\|N\|_2)^k(1-\frac{2}{k+1}) \leq \frac{4n^2\|N\|_2^2}{1-2\|N\|_2}, \\
\int_0^1 \bar{\eta}(\varepsilon)d\varepsilon &\leq \frac{4}{3}\frac{(1+n\|N\|_2)^{3/2}}{(1-2\|N\|_2)^2}\sqrt{n\|N\|_2}.
\end{aligned}$$

These estimates, together with (55) and (56) imply (45). Q.E.D.
Putting Theorem 2.1 and Theorem 3.1 together, we have

Corollary 3.2 *If $\||H|_\Delta^{-1}\|_2$ is moderate and if $\tilde{U}$ is close to the eigenvector matrix of H, then the preconditioning step is numerically feasible, at least if $\tilde{H}'$ is computed by the standard algorithm for matrix multiplication.*

Remark 3.1 The usual choice of scaling matrices $\Delta = \mathrm{diag}(|H|_{ii})^{1/2}$, $\Xi = \mathrm{diag}((\tilde{U}^*|H|\tilde{U})_{ii})^{1/2}$ is nearly optimal, see [23].

Example 3.1 We shall illustrate Theorem 3.1 by an example. We take

$$H = \begin{bmatrix} 2\cdot 10^{12} & 10^6 & 0 \\ 10^6 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} = D(E+N)D \tag{57}$$

So, this is only block s.d.d. with

$$D = \mathrm{diag}(10^6, 1, 1), \quad E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad N = \begin{bmatrix} 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

This gives (properly rounded)

$$|H|_s = \begin{bmatrix} 2.0\cdot 10^{12} & 1.0\cdot 10^6 & 6.2\cdot 10^{-7} \\ 1.0\cdot 10^6 & 1.6 & -2.4\cdot 10^{-1} \\ 6.2\cdot 10^{-7} & -2.4\cdot 10^{-1} & 9.7\cdot 10^{-1} \end{bmatrix} = D(I+N_1)D$$

with

$$N_1 = \begin{bmatrix} 2.2\cdot 10^{-16} & 5.6\cdot 10^{-1} & 4.5\cdot 10^{-13} \\ 5.6\cdot 10^{-1} & -1.1\cdot 10^{-16} & -2.0\cdot 10^{-1} \\ 4.5\cdot 10^{-13} & -2.0\cdot 10^{-1} & 0.0 \end{bmatrix}.$$

Here $\|N\|_2 = 1/\sqrt{2} \approx 0.71$ and $\|N_1\|_2 \approx 0.59$. In numerous numerical experiments with different types of randomly generated s.d.d. matrices the quotient $\|N_1\|_2/\|N\|_2$ never exceeded 1.3.

4 Using fast matrix multiplication

As we mentioned in § 1, our analysis is motivated by the problem of fast and accurate eigenvalue computation of a symmetric (generally, Hermitian) matrix H. We assume that an approximation $\tilde{U}$ of the eigenvector matrix U of H is computed by the fastest method available. If $\tilde{U}$ is a reasonable approximation of U, we expect $\tilde{H}'$ to be almost diagonal and, as a result, efficient iterative improvement using the Jacobi method. The final goal is to obtain the accuracy of the most accurate method available at a speed as close as possible to the speed of the fastest method available.

It seems reasonable to try to reduce the overhead by exploiting the possibility of matrix multiplication in less than $O(n^3)$ floating point operations. Recall that two real matrices can be multiplied in as few as $O(n^{2.376})$ floating point operations, and that algorithms of that type (Strassen's and Winograd's methods) can be found in many libraries of mathematical software. For these algorithms to be more efficient than the standard matrix multiply, the dimension n has to be large. On modern parallel computers, for large dimensions, the execution time may be $10-20\%$ less than for the standard algorithm, cf. [9]. Since in our case matrix multiplication is only a part of larger computation, the overall speedup is even smaller. Besides, fast matrix multiply algorithms are less accurate than the standard algorithm.

To illustrate the difference in accuracy between standard and fast algorithms, consider real symmetric H and real almost orthogonal $\tilde{U}$. By a result of Miller [19], a general bound

$$|\mathtt{fl}(H\tilde{U}) - H\tilde{U}| \leq f(n)\mathbf{u}|H| \cdot |\tilde{U}| + O(\mathbf{u}^2) \tag{58}$$

for a matrix multiply algorithm $\mathtt{fl}(\cdot)$ is possible only if the computation $\mathtt{fl}(H\tilde{U})$ involves at least n^3 multiplications. In other words, any algorithm that multiplies H and $\tilde{U}$ in less than n^3 multiplications cannot satisfy (58). For the class of bilinear non–commutative algorithms (this includes the Strassen's and the Winograd's algorithms), here denoted by $\mathtt{fl}_{fast}(\cdot)$, the general bound is of the form

$$\|\mathtt{fl}_{fast}(H\tilde{U}) - H\tilde{U}\|_\infty \leq g(n,\wp)\mathbf{u}\|H\|_\infty\|\tilde{U}\|_\infty, \tag{59}$$

where $\|\cdot\|_\infty$ is the ℓ_∞ norm on $\mathbf{R}^{n\times n} \simeq \mathbf{R}^{n^2}$, and $g(n,\wp)$ is a function of the dimension n and certain set of parameters $\wp$ that define the algorithm. (For the sake of simplicity we do not discuss the details here; see e.g. [11, Chapter 22].) Since $\|\tilde{U}\|_\infty \leq 1$ we obtain

$$\|\mathtt{fl}_{fast}(\tilde{U}^\tau \mathtt{fl}_{fast}(H\tilde{U})) - \tilde{U}^\tau H\tilde{U}\|_\infty \leq (2ng(n,\wp)\mathbf{u} + g(n,\wp)^2\mathbf{u}^2)\|H\|_\infty,$$

and our analysis cannot be applied because the relative error in $\tilde{H}'$ does not fit into the theory.

5 Numerical Examples

We conclude this paper with two numerical experiments. We test the LAPACK eigensolver `SSYEVD()`, the J–symmetric Jacobi eigensolver ([24], [22]) `SSYEVJ()` and the combination of `SSYEVD()` and simple two–sided Jacobi eigendecomposition on the matrix preconditioned by the eigenvectors computed by `SSYEVD()`. This hybrid procedure is denoted by `SSYEVDIJ()`. All experiments were done on an ALPHA workstation.

Example 5.1 We generate $|H| = U\Sigma U^\tau$ with $n = 500$, $\kappa_2(|H|_s) \approx 400$, $\kappa_2(|H|) \gg \kappa_2(|H|_s)$. The diagonal matrix of singular values, Σ, is chosen so that the diagonals have uniformly distributed logarithms. The matrix Σ is used to define Λ, the eigenvector matrix of H: We simply change the sign of 20 smallest Σ_{ii}. Such Λ is used to define $H = U\Lambda U^\tau$. The reference values are computed using `DSYEVJ()`, a double precision implementation of `SSYEVJ()`, and are denoted by $\lambda_{1,D} \geq \cdots \geq \lambda_{n,D}$. The eigenvalues computed by either of the single precision procedures (`SSYEVD()`, `SSYEVJ()` and `SSYEVDIJ()`) are denoted by $\lambda_{1,S} \geq \cdots \geq \lambda_{n,S}$ and the relative error is computed as

$$\text{relative error}_i = \frac{|\lambda_{i,D} - \lambda_{i,S}|}{|\lambda_{i,D}|}, \quad 1 \leq i \leq n.$$

Since $\kappa_2(|H|_s)$ in this example is moderate, the values computed by `DSYEVJ()` can be used as good reference values for testing single precision procedures. The computed relative errors are given in Figure 4. The timing results are given in Table 60.

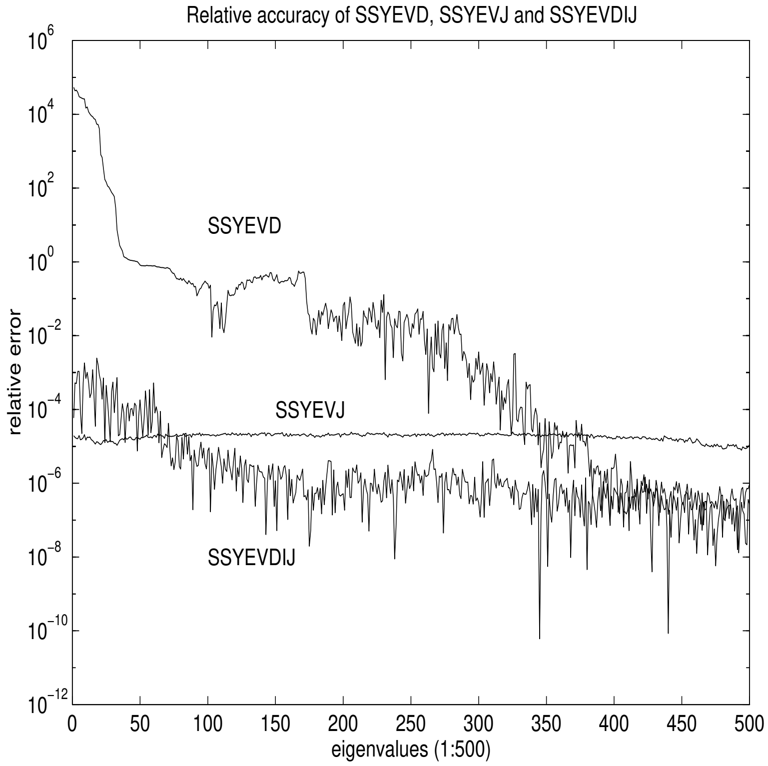

Figure 4: Relative accuracy of `SSYEVD()`, `SSYEVJ()` and `SSYEVDIJ()`

procedure	time (sec)
`SSYEVD()`	5.65
`SSYEVJ()`	24.39
`SSYEVDIJ()`	20.85

(60)

Example 5.2 In this example, H has the same dimension and the same intertia as in Example 5.1, and the eigenvalues of $|H|$ are generated as independent random numbers. The value of $\kappa_2(|H|)$ is about $7 \cdot 10^8$. The relative accuracy of `SSYEVD()`, `SSYEVJ()` and `SSYEVDIJ()` is compared in Figure 5 and the timings shown in Table 61 show a considerable speedup.

procedure	time (sec)
`SSYEVD()`	8.17
`SSYEVJ()`	37.86
`SSYEVDIJ()`	14.27

(61)

Remark 5.1 We finally note that efficient Level 3 BLAS is very important for the preconditioning step. We used `GEMM` based implementation (cf. `http://netlib.org/blas/gemm_based/` and [16], [15]) and the algorithm explained in Remark 2.2.

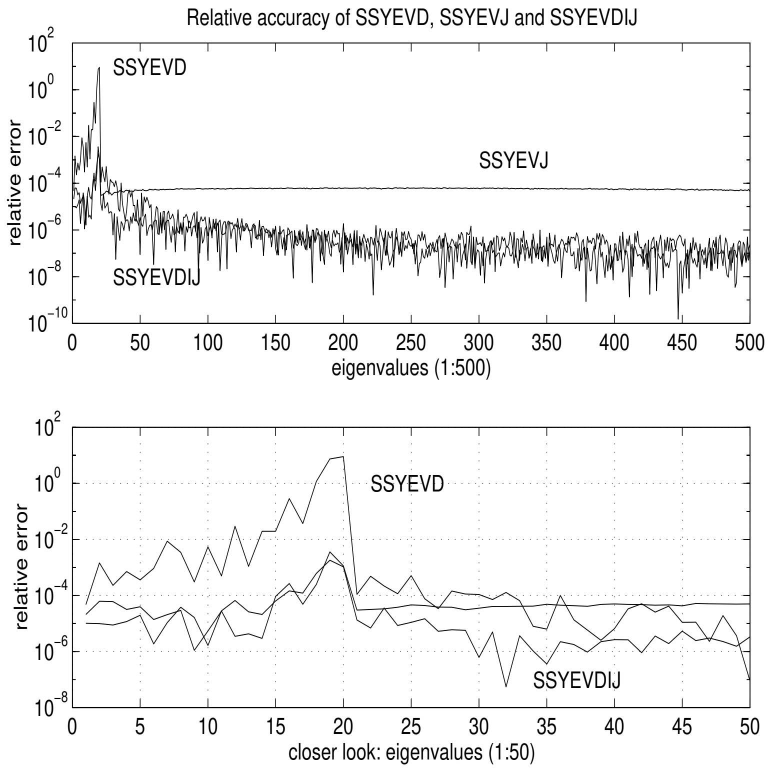

Figure 5: Relative accuracy of `SSYEVD()`, `SSYEVJ()` and `SSYEVDIJ()`

6 Appendix

In this appendix, we give the elements of the 8×8 matrix H used in Example 2.1. The matrix H is nonsingular indefinite, with three negative eigenvalues.

```
H =
  Columns 1 through 3
     8.350944166326350e+06    -3.304715861688040e+03    -6.752354724287210e+02
    -3.304715861688040e+03     2.167762629667400e-01    -2.692495376561070e-01
    -6.752354724287210e+02    -2.692495376561070e-01     4.366147385703090e-01
     1.595870930794020e+07     2.071049188867910e+03     1.788758758432980e+03
    -1.421697742711480e+00     1.779523501447970e-05     2.564775896135390e-04
    -1.314706264980880e+03    -9.635765151561029e-02     3.201425127332760e-01
    -5.748486257168610e-02     5.112662197630210e-06     8.847747042747830e-06
     2.360746434357726e+02    -1.372685785418379e-01     1.561934252809866e-02
  Columns 4 through 6
     1.595870930794020e+07    -1.421697742711480e+00    -1.314706264980880e+03
     2.071049188867910e+03     1.779523501447970e-05    -9.635765151561029e-02
     1.788758758432980e+03     2.564775896135390e-04     3.201425127332760e-01
     4.606017448740660e+07    -2.340386031341210e+00    -9.323025680468020e+01
    -2.340386031341210e+00     2.200957720795660e-07     1.568113534011200e-04
    -9.323025680468020e+01     1.568113534011200e-04    -8.882437069042130e-03
    -7.746473987422550e-03     6.506469275838140e-09     3.178147386915590e-06
     7.656960783907410e+02    -1.231861281380571e-04     5.936347580178240e-02
  Columns 7 through 8
    -5.748486257168610e-02     2.360746434357726e+02
```

```
 5.112662197630210e-06    -1.372685785418379e-01
 8.847747042747830e-06     1.561934252809866e-02
-7.746473987422550e-03     7.656960783907410e+02
 6.506469275838140e-09    -1.231861281380571e-04
 3.178147386915590e-06     5.936347580178240e-02
-1.116201295534240e-10    -3.125867993528850e-06
-3.125867993528850e-06     3.252487866740091e-02
```

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