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A projection method for the computation of inner eigenvalues using high degree rational operators

by

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Abstract

To efficiently calculate only part of the spectrum of a matrix, one can use a projection onto a suitable subspace. In this work, we present a technique to efficiently calculate such a projection without knowledge of the spectrum. The technique requires only few matrix-matrix products and inversions, which for some classes of matrices, like the $\mathcal{H}$-matrices, can be computed in almost linear complexity.

1 Introduction

Iterative techniques for determining the spectrum of a matrix like the power iteration, the QR algorithm or the Rayleigh-Ritz procedure converge fastest for the extreme spectrum, i.e., the smallest or largest eigenvalues. For an overview over the available methods for the computation of eigenvalues, e.g., the QR algorithm, see [3], or [6] for Krylov methods like the Rayleigh-Ritz procedure.

When interested in the eigenvalues in a specified interval (a, b), which may lie anywhere in the spectrum of $\mathbf{A}$, these methods may not be very efficient. One way to accelerate the convergence of such iterative schemes is to first calculate a projection $\mathbf{A}_p$ onto the space spanned by the corresponding eigenvectors. Having obtained such a projection, one can use it in a modified Rayleigh-Ritz procedure.

In this paper, we describe an efficient procedure to obtain an approximation $\tilde{\mathbf{A}}_p$ of the projection $\mathbf{A}_p$. The projection is attained without requiring prior knowledge of the spectrum of $\mathbf{A}$, except that we will assume the eigenvalues to be real. Such a projection can then be used to compute the eigenvalues in the interval (a, b) and the corresponding eigenvectors very efficiently.

A prerequisite for the efficiency is the availability of cheap matrix-matrix multiplication, matrix-inversion and application of the inverse. This is for example given by $\mathcal{H}$-matrices techniques [1], [4], [2].

In addition to using the projection to determine the eigenvalues of the matrix $\mathbf{A}$, one can use a slightly different procedure to construct the sign function, mapping the positive spectrum of $\mathbf{A}$ to 1 and the negative to -1 (cf. [5]). This will be briefly described in Section 7.

2 Prerequisites and notations

In the following, we will assume that all eigenvalues of $\mathbf{A}$ are real and that $\mathbf{A}$ possesses an orthonormal set of eigenvectors $\mathbf{V} = [v_1, \ldots, v_M]$. Consequently, $\mathbf{V}^T\mathbf{A}\mathbf{V}$ is diagonal and consists of $\mathbf{A}$'s eigenvalues, which we denote by $\lambda_1 \leq \ldots \leq \lambda_M$.

The existence of such an orthonormal matrix $\mathbf{V}$ is not necessary for the method to work. We here assume it to simplify the analysis. It is sufficient for $\mathbf{A}$ to be diagonalisable.

Given an interval (a, b), we denote the eigenvalues of $\mathbf{A}$ lying in (a, b) by $\lambda_{i+1}, \ldots, \lambda_{i+n}$ and the corresponding eigenvectors by $v_{i+1}, \ldots, v_{i+n}$. We assume that (a, b) is chosen such that no eigenvalue is exactly equal to a or b.

3 An approximation of the projection operator

Given an interval (a, b), let $\mathcal{X} : \mathbb{R} \to \mathbb{R}$ be the projection

$$\mathcal{X}(\lambda) = \begin{cases} \lambda & \text{for } \lambda \in (a, b)\,, \\ 0 & \text{otherwise.} \end{cases}$$

An approximation of the projection $\mathcal{X}$ is given by $\tilde{\mathcal{X}} : \mathbb{R} \to \mathbb{R}$

$$\tilde{\mathcal{X}}(\lambda) = \frac{\lambda}{1 + T(\lambda)^{2^\ell}} \qquad \text{with} \qquad T(\lambda) = \frac{2\lambda - (b+a)}{b-a}$$

for $\ell \in \mathbb{N}$. For large ℓ, $\tilde{\mathcal{X}}(\lambda)$ is a good approximation to the projection. To see this, we observe that for $a < \lambda < b$, $|T(\lambda)| < 1$. Thus, for large ℓ, $\tilde{\mathcal{X}}(\lambda) \approx \lambda$. On the other hand, if $\lambda > b$ or $\lambda < a$, $|T(\lambda)| > 1$, yielding $\tilde{\mathcal{X}}(\lambda) \approx 0$ for large ℓ.

The function $\tilde{\mathcal{X}}$ can be extended to matrices, in a straightforward way,

$$\begin{aligned} T(\mathbf{A}) &= (2\mathbf{A} - (b+a)\mathbf{I})/(b-a)\,, \\ \tilde{\mathbf{A}}_p := \tilde{\mathcal{X}}(\mathbf{A}) &= (\mathbf{I} + T(\mathbf{A})^{2^\ell})^{-1}\mathbf{A}\,. \end{aligned} \tag{1}$$

When applying $\tilde{\mathbf{A}}_p$ to a vector, the components in the direction of $v_{i+1}, \ldots, v_{i+n}$ remain almost unchanged while the components in the other directions are very small.

The special structure of the operator $\tilde{\mathcal{X}}$ is chosen, because it can be computed with only ℓ matrix-matrix multiplications and one matrix inversion.

In Figure 1, we give an example of the result of the operator $\tilde{\mathcal{X}}$. The eigenvalues of the original matrix $\mathbf{A}$ are depicted by crosses and the eigenvalues of $\tilde{\mathbf{A}}_p$ by diamonds. The eigenvalues close to the points a and b are mapped to values somewhere in between 0 and their original values, while the eigenvalues away from a and b are mapped almost exactly to either 0 or their original values.

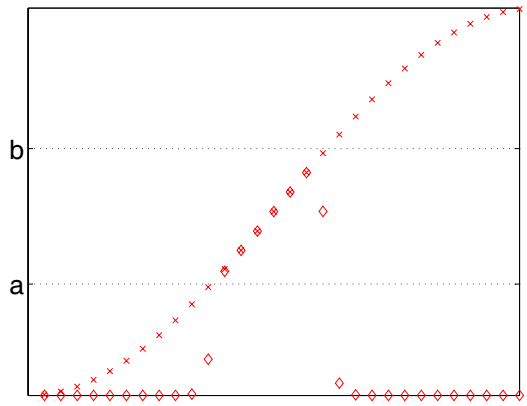


Figure 1: Spectrum of $\mathbf{A}$ (crosses) and $\tilde{\mathbf{A}}_p$ (diamonds), $\ell = 5$

One obstacle that will keep this method from working well is the observation that the entries of $\mathbf{I} + T(\mathbf{A})^{2^\ell}$ might become very large very quickly and rounding effects will make the method collapse.

Before we address this further and offer a solution to this problem, let us investigate the error $\tilde{\mathcal{X}} - \mathcal{X}$. To determine the error, we compare $\tilde{\mathcal{X}}(\lambda)$ with either λ or 0, depending on whether $\lambda \in (a, b)$ or not. First, to see how the quality of the projection of the entire matrix can be estimated by the error in the projection of the eigenvalues, we have the following lemma.

Lemma 1 *Let the eigenvalues of* $\mathbf{A}$ *be denoted by* λ_j*. For* $\lambda_j \in (a, b)$*, let* $\left|\tilde{\mathcal{X}}(\lambda_j) - \lambda_j\right| < \varepsilon$*, and for* $\lambda_j \notin (a, b)$ *let* $\left|\tilde{\mathcal{X}}(\lambda_j)\right| < \varepsilon$*. Then*

$$\left\|\mathbf{A}_p - \tilde{\mathbf{A}}_p\right\|_2 \leq \varepsilon\,,$$

where $\mathbf{A}_p = \mathcal{X}(\mathbf{A})$ *is the exact projection.*

Proof. We have $\tilde{\mathbf{A}}_p = \mathbf{V}^T diag(\tilde{\mathcal{X}}(\lambda_1), \ldots, \tilde{\mathcal{X}}(\lambda_M))\mathbf{V}$. Thus using

$$\mathbf{A}_p - \tilde{\mathbf{A}}_p = \mathbf{V}^T diag(-\tilde{\mathcal{X}}(\lambda_1), \ldots, \lambda_{i+1} - \tilde{\mathcal{X}}(\lambda_{i+1}), \ldots, \lambda_{i+n} - \tilde{\mathcal{X}}(\lambda_{i+n}), \ldots, -\tilde{\mathcal{X}}(\lambda_M))\mathbf{V}$$

and the orthogonality of $\mathbf{V}$, leads to the statement of the lemma. ■

Let us now consider the conditions on ℓ to achieve a certain accuracy ε in the approximate projection $\tilde{\mathcal{X}}(\lambda)$. An a priori estimate of the error will require some knowledge of the position of the eigenvalues close to a and b. Remember that we denoted by λ_i and λ_{i+1} the eigenvalues of $\mathbf{A}$ enclosing a and by λ_{i+n} and λ_{i+n+1} those enclosing b.

Theorem 2 *Let $\delta_j = \frac{2}{b-a}\min\{|\lambda_j - a|, |\lambda_j - b|\}$. If we choose ℓ such that*

$$2^\ell \geq \max\left\{ \frac{\log\left(\frac{\varepsilon}{|\lambda_i|-\varepsilon}\right)}{\log(\frac{1}{1+\delta_i})}, \frac{\log\left(\frac{\varepsilon}{|\lambda_{i+1}|-\varepsilon}\right)}{\log(1-\delta_{i+1})}, \frac{\log\left(\frac{\varepsilon}{|\lambda_{i+n}|-\varepsilon}\right)}{\log(1-\delta_{i+n})}, \frac{\log\left(\frac{\varepsilon}{|\lambda_{i+n+1}|-\varepsilon}\right)}{\log(\frac{1}{1+\delta_{i+n+1}})} \right\}, \tag{2}$$

then

$$\left\| \mathbf{A}_p - \tilde{\mathbf{A}}_p \right\|_2 \leq \varepsilon\,.$$

Proof. Let λ be an eigenvalue of $\mathbf{A}$. We denote by δ the distance of λ to the endpoints a and b scaled by $\frac{2}{b-a}$. If $\lambda \in (a,b)$, the error is given by

$$\left|\tilde{\mathcal{X}}(\lambda) - \lambda\right| = \frac{T(\lambda)^{2^\ell}}{1+T(\lambda)^{2^\ell}}\,|\lambda|\,.$$

The largest error is attained for values of λ close to either a or b, i.e., λ_{i+1} or λ_{i+n}. Then $T(\lambda) \leq 1-\delta$ and $|\tilde{\mathcal{X}}(\lambda) - \lambda| \leq \frac{(1-\delta)^{2^\ell}}{1+(1-\delta)^{2^\ell}}|\lambda|$. The requirement $|\tilde{\mathcal{X}}(\lambda) - \lambda| \leq \varepsilon$ leads to a lower bound on ℓ,

$$2^\ell \geq \frac{\log\left(\frac{\varepsilon}{|\lambda|-\varepsilon}\right)}{\log(1-\delta)}\,.$$

If on the other hand $\lambda \notin (a,b)$, we have

$$\left|\tilde{\mathcal{X}}(\lambda)\right| = \frac{|\lambda|}{1+T(\lambda)^{2^\ell}}\,.$$

Again, the largest error is attained for values of λ close to either a or b, i.e., λ_i or λ_{i+n+1}. Then $|T(\lambda)| \leq 1+\delta$ and $|\tilde{\mathcal{X}}(\lambda)| \leq \frac{|\lambda|}{1+(1+\delta)^{2^\ell}}$. The requirement $|\tilde{\mathcal{X}}(\lambda)| \leq \varepsilon$ leads to

$$2^\ell \geq \frac{\log\left(\frac{\varepsilon}{|\lambda|-\varepsilon}\right)}{\log(\frac{1}{1+\delta})}\,.$$

Applying Lemma 1 finishes the proof. ■

4 A preprocessing step

As mentioned above, rounding errors might cause problems in the above procedure. The matrix $\mathbf{I}+T(\mathbf{A})^{2^\ell}$ might become nearly singular. The eigenvalues of $\mathbf{I}+T(\mathbf{A})^{2^\ell}$ are $1+T(\lambda_j)^{2^\ell}$, thus they lie between 1 and $\max_{1\leq j\leq M}\left\{1+T(\lambda_j)^{2^\ell}\right\} = \max_{j=1,M}\left\{1+T(\lambda_j)^{2^\ell}\right\}$. If the condition number of $\mathbf{I}+T(\mathbf{A})^{2^\ell}$ is close to the reciprocal of machine-epsilon, $1/\varepsilon_m$, the inverse cannot be calculated with good precision. Thus, we require $\left|1+T(\lambda_j)^{2^\ell}\right| \approx |T(\lambda_j)|^{2^\ell} \leq 1/\varepsilon_m$. This leads to the requirement

$$2^\ell \leq \min\left\{ \frac{\log 1/\varepsilon_m}{\log\left|\frac{2\lambda_M-(b+a)}{b-a}\right|}, \frac{\log 1/\varepsilon_m}{\log\left|\frac{2\lambda_1-(b+a)}{b-a}\right|} \right\}. \tag{3}$$

The closer λ_M and λ_1 are to b and a, respectively, the larger we can choose ℓ. Note that with such a bound on ℓ, the achievable accuracy will depend on the extreme eigenvalues of $\mathbf{A}$. It is not desirable to have an upper

bound on ℓ that depends on the size of the largest and smallest eigenvalues of $\mathbf{A}$. In this section, we describe a preprocessing procedure that modifies the eigenvalues of $\mathbf{A}$, so that the resulting eigenvalues are closer to a and b, leaving the inner eigenvalues almost unchanged. This is done by the following operator $\tilde{\mathcal{X}}_0$, which we here give for scalars, but which can be extended to matrices in the same way as the operator $\tilde{\mathcal{X}}$.

$$T_0(\lambda) = \frac{2\lambda - (\beta+\alpha)}{\beta - \alpha}, \qquad \tilde{\mathcal{X}}_0(\lambda) = \frac{1 + T_0(\lambda)^{2^\ell}}{1 + T_0(\lambda)^{2^\ell+1}}\lambda,$$

where $\alpha < a < b < \beta$. We denote $\mathbf{A}_{new} := \tilde{\mathcal{X}}_0(\mathbf{A})$. In Figure 2, the effect of this operator is shown. It changes

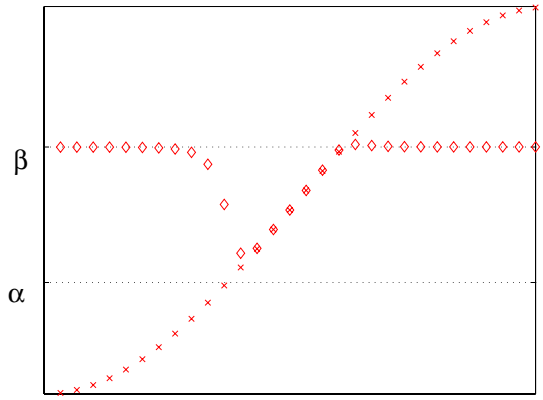


Figure 2: Spectrum of $\mathbf{A}$ (crosses) and $\mathbf{A}_{new}$ (diamonds)

the eigenvalues outside of $[\alpha, \beta)$ to β, leaving the eigenvalues in the interval (α, β) almost unchanged. Note that we have to take care in choosing α different from any eigenvalue of $\mathbf{A}$, since otherwise $\mathbf{I} + T_0(\mathbf{A})^{2^\ell+1}$ becomes singular.

The preprocessing can be used to successively dampen the eigenvalues of $\mathbf{A}$ to a region slightly larger than the interval (a, b). For this, in a first step, we only reduce the eigenvalues larger than b by choosing α considerably smaller than λ_1 and $b < \beta < \lambda_M$. We then apply the procedure to $-\mathbf{A}_{new}$, now taking $\alpha < -\lambda_{\max}(\mathbf{A}_{new})$, again considerably smaller, and $-a < \beta < -\lambda_{\min}(\mathbf{A}_{new})$. This procedure is repeated until the eigenvalues of $\mathbf{A}_{new}$ are in $[a-\eta, b+\eta]$ for sufficiently small η. Then the original procedure (1) is applied to $\mathbf{A}_{new}$.

Before we formulate the final algorithm, in the following theorem we determine the change of the eigenvalues before and after one preprocessing step. We want the eigenvalues less than β to change only slightly. Also, the eigenvalues larger than β should be mapped to a value that is very close to β.

Theorem 3 *Denote by $\lambda_- < \beta < \lambda_+$ the eigenvalues of $\mathbf{A}_{new}$ closest to β. Let $\delta_\pm = \frac{2}{\beta-\alpha}|\lambda_\pm - \beta|$. If we choose ℓ such that*

$$2^\ell \geq \max\left\{ \frac{\log \frac{\varepsilon}{\lambda_-\delta_-}}{\log(1-\delta_-)}, \frac{\log\left(\frac{\frac{\varepsilon}{\lambda_+} - 1 + \beta}{1-(\beta+\varepsilon/\lambda_+)(1+\delta_+)}\right)}{\log(1+\delta_+)} \right\}, \tag{4}$$

then for $\alpha < \lambda_1$ sufficiently small, after one preprocessing step,

$$\left\|\mathbf{A}_{new}^{exact} - \mathbf{A}_{new}\right\|_2 \leq \varepsilon,$$

where $\mathbf{A}_{new}^{exact} = \mathbf{V}^T diag(\lambda_1, \ldots, \lambda_-, \beta, \ldots, \beta)\mathbf{V}$ is the matrix, where all eigenvalues greater than β are replaced by β.

Proof. The error will be maximal for those eigenvalues close to α and β. When choosing α sufficiently small, the error will be maximal for the eigenvalues close to β. Let λ be an eigenvalue of $\mathbf{A}$. Then for $\lambda < \beta$, the

error is determined by

$$\tilde{\mathcal{X}}_0(\lambda) - \lambda = \frac{T_0(\lambda)^{2^l}\,(1 - T_0(\lambda))\,\lambda}{1 + T_0(\lambda)^{2^\ell+1}}\,.$$

The error is largest for λ close to β. Consider $\lambda_- = \beta - \frac{(\beta-\alpha)\delta_-}{2}$. The requirement

$$|\tilde{\mathcal{X}}_0(\lambda_-) - \lambda_-| = \frac{(1-\delta_-)^{2^\ell}\delta_-}{1 + (1-\delta_-)^{2^\ell+1}}\lambda_- \leq \varepsilon$$

leads to

$$\begin{aligned}(1-\delta_-)^{2^\ell}\delta_- &\leq \frac{\varepsilon}{\lambda_-}\left(1 + (1-\delta_-)^{2^\ell+1}\right) \approx \frac{\varepsilon}{\lambda_-}\\ \Rightarrow \qquad 2^\ell &\geq \frac{\log\frac{\varepsilon}{\lambda_-\delta_-}}{\log(1-\delta_-)}\,.\end{aligned}$$

For $\lambda > \beta$, the error is determined by considering the deviation of the new eigenvalues from β:

$$\tilde{\mathcal{X}}_0(\lambda) - \beta = \frac{(1 + T_0(\lambda)^{2^\ell} - \beta(1 + T(\lambda)^{2^\ell+1}))\lambda}{1 + T(\lambda)^{2^\ell+1}}\,.$$

The largest error is attained for $\lambda_- = \beta + \frac{(\beta-\alpha)\delta_-}{2}$ where we have $T(\lambda_+) = 1 + \delta_+$ and

$$\begin{aligned}\mathcal{X}(\lambda_+) - \beta &= \frac{(1 + (1+\delta_+)^{2^\ell} - \beta(1 + (1+\delta_+)^{2^{\ell+1}}))}{1 + (1+\delta_+)^{2^\ell+1}}\lambda_+ \leq \varepsilon\\ \Rightarrow \qquad 2^\ell &\geq \frac{\log\left(\frac{\frac{\varepsilon}{\lambda_+}-1+\beta}{1-(\beta+\varepsilon/\lambda_+)(1+\delta_+)}\right)}{\log(1+\delta_+)}\,.\end{aligned}$$

Again, a similar reasoning as in Lemma 1 yields the statement of the lemma. ■

Again, to avoid rounding and cancellation, we require

$$2^\ell \leq \frac{\log 1/\varepsilon_m}{\log\left|\frac{2\lambda_{\max}(\mathbf{A})-(\beta+\alpha)}{\beta-\alpha}\right|}\,. \tag{5}$$

The above error estimates have assumed exact inversion and application of the inverse. In $\mathcal{H}$-matrix techniques, the inverse is only calculated approximately, and the matrix-matrix multiplication results in an error. If we assume that the matrix inversion and matrix-matrix multiplication is performed with an error ε, the additional error in each preprocessing step is bounded by $(2\ell+5)\varepsilon$ and the additional error in the final step is bounded by $(\ell+4)\varepsilon$. We are now ready to give the complete projection algorithm including preprocessing steps.

```
Anew := A;
while β − b > η or a − α > η do
begin choose α, β with α < λmin(Anew), b < β < λmax(Anew);
    choose ℓ according to (4), (5) ;
    Anew := - preproc(Anew,α,β,ℓ);
    choose α, β with α < λmin(Anew), b < β < λmax(Anew);
    choose ℓ according to (4), (5) ;
    Anew := - preproc(Anew,α,β,ℓ)
end;
choose ℓ according to (2), (3);
Anew := final(Anew,a,b,ℓ);
```

with the functions

size $\mathbf{A}$	a	b	η^*	η	$\max \frac{\lambda_{new}-\lambda_{proj}}{\lambda}$	$\#M \cdot M$	$\#M^{-1}$
30×30	11.5	25.5	0.308	3.08	$2.7e-02$	34	6
				1.26	$1.8e-02$	57	9
				0.616	$4.85e-06$	74	11
				0.308	$1.17e-06$	93	13
	2.5	12.5	0.013	0.105	$1.45e-02$	117	15
				0.055	$1.0e-03$	129	16
				0.026	$1.97e-05$	167	19
100×100	11.5	25.5	0.22	3.08	$7.4e-02$	34	6
				1.26	$8.8e-03$	57	9
				0.616	$1.48e-04$	74	11
				0.308	$1.11e-06$	93	13
	2.5	12.5	0.074	0.105	$1.79e-05$	117	15
				0.055	$1.29e-06$	129	16
				0.026	$1.71e-05$	167	19

Table 1: Approximate projection of $\mathbf{A}$

```
function preproc(A,α,β,ℓ)
begin Atemp := (2*A - (β + α)*I)/(β − α);
   Atemp2 := Atemp*Atemp;
   for i = 2 to ℓ do Atemp2 := Atemp2*Atemp2;
   preproc := invers(I + Atemp2*Atemp)*(I + Atemp2)*A
end;

function final(A,α,β,ℓ)
begin Atemp := (2*A - (β + α)*I)/(β − α);
   Atemp2 := Atemp*Atemp;
   for i = 2 to ℓ do Atemp2 := Atemp2*Atemp2;
   final := invers(I + Atemp2)*A
end;
```

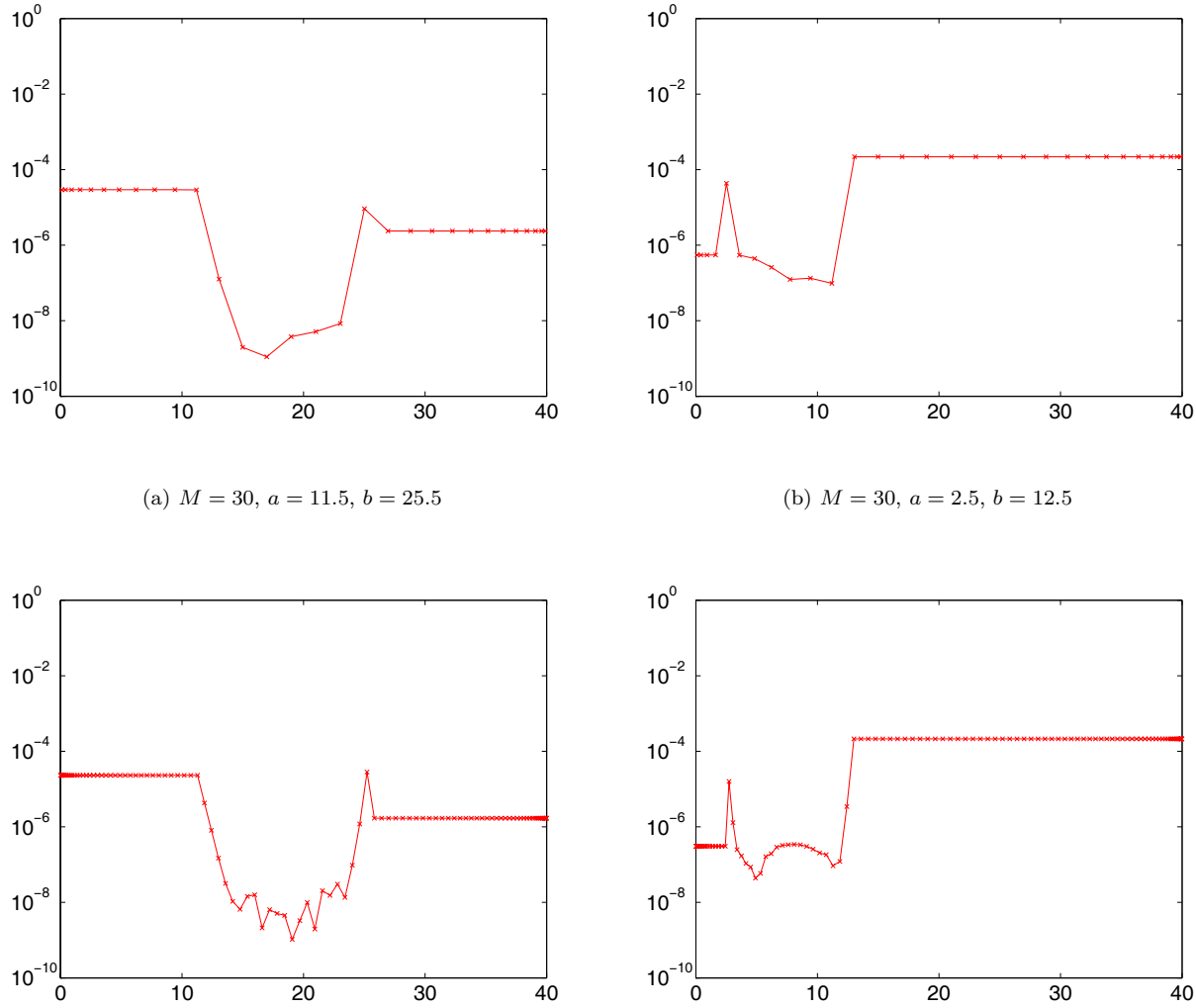
5 Numerical experiments

We test the procedure for the $M \times M$ matrix

$$\mathbf{A} = 10 \cdot \begin{pmatrix} 2 & -1 & 0 & \cdots \\ -1 & 2 & -1 & 0 \\ \ddots & \ddots & \ddots & \ddots \\ \cdots & 0 & -1 & 2 \end{pmatrix}.$$

Its eigenvalues lie between 0 and 40.

For the preprocessing, we choose $\beta = b + \frac{\lambda_{\max}(\mathbf{A})-b}{2}$, i.e., we decrease the distance between b and the largest eigenvalue of $\mathbf{A}$ by a factor 2, and $\alpha = \lambda_{\min}(\mathbf{A}) - \frac{b-a}{2}$. We continue with the preprocessing until $\beta = b+\eta$. The results of the numerical tests are summarized in Table 1. We chose two different values for M to investigate the performance of the method when the distance of the eigenvalues to a and b decreases. We performed tests for two different values of a and b. In the table, η^* denotes the distance of the original eigenvalues to a and b (this distance determines the smallest value for η we should choose for the preprocessing). In the fifth column, we give the largest relative error compared to the exact projection. The factor ℓ is chosen as large as possible and the seventh and eighth columns give the number of matrix-matrix multiplications required, and the number of matrix inversions, respectively. In Figure 3, we depict the relative error of the projection by showing the error in the eigenvalues, where on the x-axis, the original eigenvalues are shown.



(a) $M = 30$, $a = 11.5$, $b = 25.5$

(b) $M = 30$, $a = 2.5$, $b = 12.5$

(c) $M = 100$, $a = 11.5$, $b = 25.5$

(d) $M = 100$, $a = 2.5$, $b = 12.5$

Figure 3: Relative error in the eigenvalues

6 Modified Rayleigh-Ritz procedure

We have presented a method to obtain an approximate projection of $\mathbf{A}$ onto the space of eigenvectors corresponding to eigenvalues inside an interval (a, b). As mentioned in the introduction, this projection can be used in a modified Rayleigh-Ritz procedure to determine the eigenvalues of $\mathbf{A}$ inside (a, b).

For this let $U_k = [u_1, \ldots, u_k]$ be orthonormal and its columns span a subspace of the image of $\tilde{\mathbf{A}}_p$. The vectors u_i can be obtained by starting with a random vector u_0, and we obtain u_i from orthonormalising the space spanned by $\tilde{\mathbf{A}}_p u_0, \ldots, \tilde{\mathbf{A}}_p^k u_0$. Consider now the $k \times k$ matrix $S_k = U_k^T \mathbf{A} U_k$. Its eigenvalues and eigenvectors are called Ritz values and Ritz vectors. For increasing k, the Ritz values converge towards the eigenvalues of $\mathbf{A}$ in the interval (a, b) and applying U_k to the Ritz vectors will yield approximate eigenvectors of $\mathbf{A}$. Thus in order to obtain approximate eigenvalues of $\mathbf{A}$ in the interval (a, b), it is sufficient to find the eigenvalues of the usually much smaller matrix S_k.

7 Sign function

Defining $\mathbf{P}_A := (\mathbf{I} + T(\mathbf{A})^{2^\ell})^{-1}$, with $T(\mathbf{A})$ as in (1), gives an operator that maps the eigenvalues in (a, b) to 1 and the eigenvalues outside of (a, b) to 0. We can use the operators $\mathbf{P}_+$ and $\mathbf{P}_+$, defined by taking $a = 0$ and $b > \lambda_M$ for $\mathbf{P}_+$ and $a < \lambda_1$ and $b = 0$ for $\mathbf{P}_-$, to construct an approximation to the sign function

$$\operatorname{sign}(\mathbf{A}) = \mathbf{P}_+ - \mathbf{P}_-$$

which maps the positive spectrum to 1 and the negative to -1.

8 Concluding Remarks

The procedure gives very good results for the eigenvalues that are not too close to a or b, respectively. One strategy can be to choose the interval (a, b) slightly larger than what is desired, and when we have computed the Ritz values using the matrix $\tilde{\mathbf{A}}_p$, we discard the extreme ones. The above error analysis can then be relaxed considerably.

A prerequisite for the efficiency is the availability of cheap matrix-matrix multiplication, matrix-inversion and application of the inverse. This is for example given by $\mathcal{H}$-matrices techniques [4], [2].

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