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Improving the numerical stability of the Sakurai-Sugiura method for quadratic eigenvalue problems

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1. Introduction

We consider quadratic eigenvalue problems (QEPs)

\[ Q(\lambda) x = (\lambda^2 A_2 + \lambda A_1 + A_0) x = 0, \tag{1} \]

where \( A_2, A_1, A_0 \in \mathbb{C}^{n \times n} \setminus \{0\} \), and \( \lambda \in \mathbb{C} \) and \( x \in \mathbb{C}^n \setminus \{0\} \) are eigenvalues and their associated eigenvectors.

QEPs appear naturally in modal analysis of physical structures [1]. In certain applications such as structural dynamics and structural-acoustic interactions, only a partial set of eigenpairs \((\lambda, x)\) is desired.

The Sakurai-Sugiura method has been proposed as an efficient method for computing a subset of eigenpairs of generalized eigenvalue problems [2] and of quadratic eigenvalue problems [3]. The Sakurai-Sugiura method with Rayleigh-Ritz procedure (SS-RR method) can extract eigenvalues inside a Jordan curve \( \Gamma \) using a subspace constructed by a contour integral approach. In the SS-RR method, \( Q(\lambda) \) is projected into a quadratic matrix polynomial

\[ R(\lambda) = V^H Q(\lambda) V = \lambda^2 R_2 + \lambda R_1 + R_0 \tag{2} \]

of smaller dimension, where the matrix \( V \in \mathbb{C}^{n \times n} \), \( m < n \), has orthonormal columns consisting of basis vectors for the subspace constructed by the SS-RR method. Then the pair \((\lambda, \tilde{y})\) is taken as approximate eigenpair for \( Q(\lambda) \), where \((\lambda, y)\) is an approximate eigenpair of \( R(\lambda) \). However, unless special care is taken when solving the projected QEP \( R(\lambda) y = 0 \), the SS-RR method can suffer from numerical instability when the coefficient matrices \( R_i, i = 0, 1, 2 \), of \( R(\lambda) \) vary widely in norm (for example when \( \|R_0\|_2 \gg \|R_2\|_2 \) and \( \|R_2\|_2 \gg \|R_1\|_2 \)).

Our aim is to show that solving the projected QEP (2) with a numerically stable eigensolver is crucial for the numerical stability of the SS-RR method.

The remainder of this paper is organized as follows. In Section 2, we give a brief description of the SS-RR method. In Section 3, we describe an eigensolver for the complete solution of QEPs and discuss its backward stability. In Section 4, we investigate the backward stability of the SS-RR method. In Section 5, we present numerical experiments that confirm our results. Finally, our conclusions are presented in Section 6.

2. The SS-RR method for QEPs

The SS-RR method computes eigenvalues located inside a Jordan curve \( \Gamma \) as follows. Here, we assume that \( Q(\lambda) \) has no eigenvalues on \( \Gamma \). Given two positive integers \( K \) and \( L \), define

\[ S = [S_0, \ldots, S_{K-1}] \in \mathbb{C}^{n \times KL}, \]

where

\[ S_k = \frac{1}{2\pi i} \int_{\Gamma} g_k(z) Q(z)^{-1} U dz \in \mathbb{C}^{n \times L}, \tag{3} \]

with \( g_k \) a \( k \)-th degree polynomial function and \( U \) an \( n \times L \) matrix of full rank. Since the target eigenvectors of \( Q(\lambda) \) belong to \( \text{span}\{S\} \), the target eigenpairs of \( Q(\lambda) \) can be computed by the Rayleigh-Ritz procedure with projection onto \( \text{span}\{S\} \).

Numerical quadrature is used to approximate the contour integral in (3). The approximation of \( S_k \) is then
Algorithm 1 SS-RR method

**Input:** $N, K, L \in \mathbb{N}^+, U \in \mathbb{C}^{n \times L}$, $z_p, \omega_p, p = 1, \ldots, N$, a Jordan curve $\Gamma$, and a quadratic matrix polynomial $Q(\lambda)$.

**Output:** $\tilde{\lambda}_j, \tilde{\omega}_j, j = 1, \ldots, n(\Gamma)$, where $n(\Gamma)$ is the number of eigenvalues of $Q(\lambda)$ inside $\Gamma$.

1. Compute $Q(z_p)^{-1}U$, $p = 1, \ldots, N$.
2. Compute $\tilde{S}_k$, $k = 0, \ldots, K-1$ using (4).
3. Compute the singular value decomposition $\tilde{S} = V \Sigma W^H$, where $V = [\tilde{S}_0, \ldots, \tilde{S}_{K-1}]$.
4. Set $V = \tilde{V}(:, 1: m)$, where $m$ is the numerical rank of $\tilde{S}$.
5. Compute the eigenpairs $(\tilde{\lambda}_j, \tilde{\omega}_j)$, $j = 1, \ldots, m$ of $R(\lambda) = V^H Q(\lambda) V$.
6. Extract the $n(\Gamma)$ eigenvalues of $\lambda_j$, $j = 1, \ldots, n(\Gamma)$ that are inside $\Gamma$ and set $\tilde{x}_j = V \tilde{y}_j, j = 1, \ldots, n(\Gamma)$.

provided by

$$S_k \approx \tilde{S}_k = \sum_{p=1}^{N} \omega_p g_k(z_p)Q(z_p)^{-1} U,$$

where $z_p$ and $\omega_p$, $p = 1, \ldots, N$, are quadrature points and their associated weights.

A low-rank approximation of $\tilde{S} = [\tilde{S}_0, \ldots, \tilde{S}_{K-1}]$ is constructed by computing the singular value decomposition of $\tilde{S}$ as

$$\tilde{S} = V \Sigma W^H \approx V \Sigma W^H,$$

where $V = \tilde{V}(:, 1: m)$ and $m$ is the numerical rank of $\tilde{S}$. The matrix $V$ is then used to reduce $Q(\lambda)$ into $R(\lambda)$ as in (2). The eigenpairs of $Q(\lambda)$ are approximated by

$$(\tilde{\lambda}_j, \tilde{\omega}_j) = (\lambda_j, V \tilde{y}_j), j = 1, \ldots, m,$$

where $(\lambda_j, \tilde{y})$, $j = 1, \ldots, m$ are the computed eigenpairs of $R(\lambda)$.

The main steps of the SS-RR method are summarized in Algorithm 1.

3. Eigensolvers for the complete solution of QEPs

We now discuss why the numerical solution of the QEP in step 5 requires special attention. The standard way of solving small to medium size dense QEPs,

$$R(\lambda)y = (\lambda^2 R_2 + \lambda R_1 + R_0)y = 0,$$

is via linearization. We assume $R_2, R_1, R_0 \in \mathbb{C}\{O\}$. This consists of rewriting (5) as a generalized eigenvalue problem (GEP) $L(\lambda)v = 0$ of twice the dimension, where for example,

$$L(\lambda) = \lambda \begin{bmatrix} R_2 & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} R_1 & R_0 \\ -I & 0 \end{bmatrix}, \quad v = \begin{bmatrix} \lambda y \\ y \end{bmatrix},$$

then solve the GEP with the QZ algorithm, and finally recover the eigenvectors $y$ of $Q(\lambda)$ from the eigenvectors $v$ of $L(\lambda)$.

Despite the fact that the QZ algorithm is backward stable for GEPs, it can be backward unstable for QEPs, in particular when the norms of the coefficient matrices of $R(\lambda)$ vary widely [4]. As a result, the computed eigenpairs of $Q(\lambda)$ may not be the exact eigenpairs of a nearby quadratic.

Scaling of the eigenvalue parameter (e.g., $\lambda = \gamma \mu$, $\mu$ being the new eigenvalue) has been shown to improve the backward stability of the solution process [5–7]. Such scaling has been implemented in the eigensolver quadeig [8]. The latter offers three types of eigenvalue parameter scalings:

- Fan, Lin, and Van Dooren scaling: $\gamma_{F-LV} = \sqrt{\|R_0\|_2}$
- tropical scaling with largest root, $\gamma_{trop}^+$
- tropical scaling with smallest root, $\gamma_{trop}^-$

The Fan, Lin, and Van Dooren scaling [7] is employed by default in quadeig for QEPs that are not too heavily damped, i.e., when

$$\|R_1\|_2 \leq \sqrt{\|R_2\|_2 \|R_0\|_2}.$$  

In that case, an eigenpair $(\tilde{\lambda}, \tilde{y})$ computed by quadeig is guaranteed to have a small backward error. Recall from [4] that the backward error of an approximate eigenpair $(\hat{\lambda}, \hat{y})$ of $R(\lambda)$ in (2) can be defined by

$$\eta(R, \hat{\lambda}, \hat{y}) := \min(\epsilon : (R(\hat{\lambda}) + \Delta R(\hat{\lambda}))\hat{y} = 0,$$

$$\|\Delta R\|_2 \leq \epsilon \|R_i\|, \quad i = 0, 1, 2),$$

where $\Delta R(\lambda) = \lambda^2 \Delta R_2 + \lambda \Delta R_1 + \Delta R_0$ is a perturbation of $R(\lambda)$.

For heavily damped QEPs, it follows from [9, Thm. 2] that when $R_2$ and $R_1$ are well conditioned, $\gamma_{trop}^+$ is small enough then there are precisely $m$ eigenvalues of the $m \times m$ quadratic matrix polynomial $R(\lambda)$ with moduli of the order of $\gamma_{trop}^+$. Similarly, when $R_1$ and $R_0$ are both well conditioned, the moduli of the $m$ smallest eigenvalues of $R(\lambda)$ are close to the smallest tropical root $\gamma_{trop}^-$. Then quadeig with tropical scaling with largest root (respectively smallest root) guarantees to return computed eigenpairs $(\hat{\lambda}, \hat{y})$ with small backward errors for those eigenvalues $\hat{\lambda}$ of moduli close to $\gamma_{trop}^+$ (respectively, $\gamma_{trop}^-$).

Based on the above comments, we propose to use quadeig in step 5 of Algorithm 1 to solve the projected QEP $R(\lambda)y = 0$. We use the Fan, Lin and Van Dooren scaling for not too heavily damped QEPs, i.e., when the matrix coefficients of $R(\lambda)$ satisfy (6). For heavily damped QEPs, we use tropical scaling: we choose $\gamma_{trop}^+$ if we are interested in the eigenvalues of large magnitude and $\gamma_{trop}^-$ otherwise.

Note that we could have used the backward stable eigensolver for QEPs presented in [10], but the latter is not freely available unlike quadeig.

4. Analysis of the backward errors of eigenpairs computed by Algorithm 1

In this section, we investigate why the use of a backward stable eigensolver in step 5 of Algorithm 1 improves the backward stability of the SS-RR algorithm. We will
make use of the explicit and computable expression for the backward error \( \eta(R, \tilde{\lambda}, \tilde{y}) \) given in [4]:

\[
\eta(R, \tilde{\lambda}, \tilde{y}) = \frac{\|R(\tilde{\lambda})\tilde{y}\|_2}{\|\sum_{i=0}^{\infty} \| R_i \|_2 \| \tilde{y} \|_2}.
\]

(7)

Let \((\tilde{\lambda}, \tilde{y})\) and \((\hat{\lambda}, \hat{y})\) be approximations to the same eigenpair \((\lambda, y)\) of \(R(\lambda)\) in (2). Assume that \((\hat{\lambda}, \hat{y})\) computed by a stable eigensolver and \((\tilde{\lambda}, \tilde{y})\) computed by an unstable eigensolver are such that

\[
\eta(R, \tilde{\lambda}, \tilde{y}) \leq \eta(R, \hat{\lambda}, \hat{y}).
\]

(8)

In what follows we identify a sufficient condition under which (8) implies that

\[
\eta(Q, \check{\lambda}, V \hat{y}) \leq \eta(Q, \check{\lambda}, V \tilde{y}).
\]

(9)

We will need the following lemma.

**Lemma 1** Let \((\check{\lambda}, \check{y})\) be a non exact approximate eigenpair of \(R(\lambda)\) in (2) with \(\check{y}\) normalized so that \(\|\check{y}\|_2 = 1\). Then for the approximate eigenpair \((\tilde{\lambda}, \tilde{y})\) of \(Q(\lambda)\) we have

\[
L_1(\check{\lambda}) \eta(R, \check{\lambda}, \check{y}) \leq \eta(Q, \check{\lambda}, V \check{y}) \leq L_2(\tilde{\lambda}) \eta(R, \tilde{\lambda}, \tilde{y}),
\]

where

\[
L_1(\check{\lambda}) := \frac{\sum_{i=0}^{\infty} \| R_i \|_2}{\sum_{i=0}^{\infty} \| A_i \|_2},
\]

\[
L_2(\tilde{\lambda}) := \frac{\|Q(\check{\lambda})V \check{y}\|_2}{\|R(\check{\lambda})\check{y}\|_2}.
\]

**Proof.** This follows directly from (7) and \(\|V \check{y}\|_2 = \|\check{y}\|_2 = 1\). Note that \(\|R(\check{\lambda})\check{y}\|_2 \neq 0\) since \((\check{\lambda}, \check{y})\) is not an eigenpair of \(R(\lambda)\). \(\Box\)

Based on Lemma 1, we have the following theorem.

**Theorem 2** Let \((\check{\lambda}, \check{y})\) and \((\hat{\lambda}, \hat{y})\) be non exact approximations to an eigenpair \((\lambda, y)\) of the QEP \(R(\lambda)\) in (2). Let \(\alpha \geq 1\) be such that \(\eta(R, \check{\lambda}, \check{y}) = \alpha \eta(R, \hat{\lambda}, \hat{y})\) and let the functions \(L_1, L_2\) be defined as in Lemma 1. If

\[
\kappa := \alpha L_1(\check{\lambda})/L_2(\tilde{\lambda}),
\]

(10)

then the inequality (9) holds for the approximate eigenpairs \((\check{\lambda}, V \check{y})\) and \((\hat{\lambda}, V \hat{y})\) of \(Q(\lambda)\).

**Proof.** Based on Lemma 1, we have

\[
\eta(Q, \check{\lambda}, V \check{y}) \geq L_1(\check{\lambda}) \eta(R, \check{\lambda}, \check{y}) \geq \alpha \eta(R, \hat{\lambda}, \hat{y}) \geq \kappa \eta(Q, \tilde{\lambda}, V \tilde{y}).
\]

The inequality (9) holds because \(\kappa \geq 1\). \(\Box\)

Let us examine the condition in (10). It is easy to show that \(L_1(\check{\lambda}) \leq 1\) and that \(L_2(\tilde{\lambda}, \tilde{y}) \geq 1\) so that \(L_1(\check{\lambda})/L_2(\tilde{\lambda}, \tilde{y}) \leq 1\). But if the projection \(V\) does not change much the norms of the coefficient matrices of \(Q(\lambda)\), that is, \(\|A_i\|_2 \approx \|V^H A_i V\|_2\) then \(L_1(\check{\lambda}) \approx 1\). Also, if the norm of the residual for the approximate eigenpair \((\lambda, y)\) of \(R(\lambda)\) is small then we can expect the norm of the residual \(Q(\lambda)V \hat{y}\) to be small as well so that \(L_2(\tilde{\lambda}, \tilde{y}) \approx 1\). Since \(\alpha \geq 1\) then (9) is likely to hold. So what Theorem 2 says is that if we can improve the backward error for the approximate eigenpairs of \(R(\lambda)\) then we can improve the backward error for the approximate eigenpairs of \(Q(\lambda)\). This justifies the use of a numerically stable eigensolver in step 5 of Algorithm 1.

5. Numerical experiments

We now compare the numerical stability of the SS-RR method with either quadeig and the choice of scaling discussed in Section 3 or polyeig to perform step 5 of Algorithm 1. The MATLAB function polyeig solves polynomial eigenvalue problems of arbitrary degree and hence is more general than quadeig. However, it does not employ any scaling and can suffer from numerical instability. All the computations are performed using MATLAB 2015.

The test problems listed in Table 1 are QEPs belonging to the collection of nonlinear eigenvalue problems NLEV [11] and are selected so as to have large variations in the norms of their coefficient matrices. The mod.spring and mod.sleeper problems correspond to the spring and sleeper problems in [11] but with the damping matrix \(A_1\) multiplied by \(10^2\).

For each problem, the Jordan curve \(\Gamma\) is a circle of center \(c\) and radius \(r\), whose values are given in Table 2. For the parameters \(N, K, L\) we use \(N = 32, K = 8\) and \(L = 16\). For the quadrature points and corresponding weights we use

\[
z_p = c + r \exp\left(\frac{2\pi i(p-1/2)}{N}\right),
\]

\[
\omega_p = \frac{(z_p - c)}{N}, \quad p = 1, \ldots, N.
\]

As shown in Table 3, the norms of the coefficient matrices of the projected problems vary widely. The projected damped_beam and wiresaw2 problems are not too heavily damped since \(\|V^H A_1 V\|_2 \leq \|V^H A_2 V\|_2\). Hence, for these two problems, quadeig is called with the Fan, Lin and Van Dooren scaling \(\gamma_{FLV}\). The projected mod.spring and mod.sleeper are overdamped. Since we are interested in computing eigenvalues of magnitude around \(10^3\) for these two problems (see Table 2), quadeig is called with tropical scaling with largest root \(\gamma_{top}\) (Table 4 shows that \(\gamma_{top} \approx 10^3\) for both problems). With this choice of scalings, quadeig guarantees to return eigenpairs \((\lambda, y)\) inside \(\Gamma\) with backward errors \(\eta(R, \tilde{\lambda}, \tilde{y}) \leq \nu u\), where \(u\) is the machine precision. For these problems, polyeig returns eigenpairs \((\lambda, y)\) with \(\eta(R, \tilde{\lambda}, \tilde{y}) \gg \nu u\) so that (8) holds.

Table 4 displays the smallest value \(\kappa_{\text{min}}\) of \(\kappa\) in (10), where \(\tilde{\lambda}\) corresponds to eigenvalues computed by polyeig and \((\lambda, y)\) are the corresponding eigenpairs computed by quadeig. Table 4 shows that the assumption \(\kappa > 1\) is satisfied for all the problems. It then follows from Theorem 2 that the inequality (9) holds between eigenpairs from SS-RR with quadeig and SS-RR with...
This is confirmed by the backward error results presented in Table 5, Fig. 1, and Fig. 2. They also show that the SS-RR method with 
*quadeig* and appropriate scaling computes eigenpairs \((\tilde{\lambda}, V \tilde{y})\) with backward errors \(\eta(Q, \tilde{\lambda}, V \tilde{y})) \lesssim \eta u\), which is the best we can expect.

### 6. Conclusion

We have shown that to improve the backward stability of the SS-RR method, it is crucial to combine it with a backward stable algorithm for the complete solution of the projected QEP. In future work, we plan to investigate the inclusion of scaling techniques in other types of Sakurai-Sugiura methods.

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