

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

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Abstract

The Sakurai-Sugiura method with Rayleigh-Ritz projection (SS-RR method) finds the eigenvalues in a certain domain of the complex plane of large quadratic eigenvalue problems (QEPs). The SS-RR method can suffer from numerical instability when the coefficient matrices of the projected QEP vary widely in norm. To improve the numerical stability of the SS-RR method, we combine it with a numerically stable eigensolver for the small projected QEP. We analyze the backward stability of the proposed method and show, through numerical experiments, that it computes eigenpairs with backward errors that are smaller than those computed by the SS-RR method.

Keywords SS-RR method, quadratic eigenvalue problem, backward error

Research Activity Group Algorithms for Matrix / Eigenvalue Problems and their Applications

1. Introduction

We consider quadratic eigenvalue problems (QEPs)

$$Q(\lambda)\mathbf{x} = (\lambda^2 A_2 + \lambda A_1 + A_0)\mathbf{x} = \mathbf{0}, \quad (1)$$

where $A_2, A_1, A_0 \in \mathbb{C}^{n \times n} \setminus \{O\}$, and $\lambda \in \mathbb{C}$ and $\mathbf{x} \in \mathbb{C}^n \setminus \{\mathbf{0}\}$ 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 (λ, \mathbf{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 Γ using a subspace constructed by a contour integral approach. In the SS-RR method, $Q(\lambda)$ is projected into a quadratic matrix polynomial

$$R(\lambda) = V^H Q(\lambda) V = \lambda^2 R_2 + \lambda R_1 + R_0 \quad (2)$$

of smaller dimension, where the matrix $V \in \mathbb{C}^{n \times m}$, $m \ll n$, has orthonormal columns consisting of basis vectors for the subspace constructed by the SS-RR method. Then the pair $(\hat{\lambda}, V\hat{\mathbf{y}})$ is taken as approximate eigenpair for $Q(\lambda)$, where $(\hat{\lambda}, \hat{\mathbf{y}})$ is an approximate eigenpair of $R(\lambda)$. However, unless special care is taken when solving the projected QEP $R(\lambda)\mathbf{y} = \mathbf{0}$, 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 Γ as follows. Here, we assume that $Q(\lambda)$ has no eigenvalues on Γ . Given two positive integers K and L , define

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

where

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

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

Output: $\hat{\lambda}_j, \hat{\mathbf{x}}_j, j = 1, \dots, n(\Gamma)$, where $n(\Gamma)$ is the number of eigenvalues of $Q(\lambda)$ inside Γ .

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

$$S_k \approx \hat{S}_k = \sum_{p=1}^N \omega_p g_k(z_p) Q(z_p)^{-1} U, \quad (4)$$

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

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

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

where $V = \hat{V}(:, 1:m)$ and m is the numerical rank of \hat{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

$$(\hat{\lambda}_j, \hat{\mathbf{x}}_j) = (\hat{\lambda}_j, V \hat{\mathbf{y}}_j), \quad j = 1, \dots, m,$$

where $(\hat{\lambda}_j, \hat{\mathbf{y}}_j), j = 1, \dots, m$ 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,

$$R(\lambda) \mathbf{y} = (\lambda^2 R_2 + \lambda R_1 + R_0) \mathbf{y} = \mathbf{0}, \quad (5)$$

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

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

then solve the GEP with the QZ algorithm, and finally recover the eigenvectors \mathbf{y} of $R(\lambda)$ from the eigenvectors \mathbf{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:
 $\gamma_{FLV} = \sqrt{\|R_0\|_2 / \|R_2\|_2}$,
- tropical scaling with largest root,
 $\gamma_{trop}^+ = \|R_1\|_2 / \|R_2\|_2$,
- tropical scaling with smallest root,
 $\gamma_{trop}^- = \|R_0\|_2 / \|R_1\|_2$.

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

$$\|R_1\|_2 \leq \sqrt{\|R_2\|_2 \|R_0\|_2}. \quad (6)$$

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

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

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

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, and $\gamma_{trop}^- / \gamma_{trop}^+$ 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 γ_{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 γ_{trop}^- . Then `quadeig` with tropical scaling with largest root (respectively smallest root) guarantees to return computed eigenpairs $(\hat{\lambda}, \hat{\mathbf{y}})$ with small backward errors for those eigenvalues $\hat{\lambda}$ of moduli close to γ_{trop}^+ (respectively, γ_{trop}^-).

Based on the above comments, we propose to use `quadeig` in step 5 of Algorithm 1 to solve the projected QEP $R(\lambda) \mathbf{y} = \mathbf{0}$. 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 γ_{trop}^+ if we are interested in the eigenvalues of large magnitude and γ_{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 $\eta(R, \hat{\lambda}, \hat{\mathbf{y}})$ given in [4]:

$$\eta(R, \hat{\lambda}, \hat{\mathbf{y}}) = \frac{\|R(\hat{\lambda})\hat{\mathbf{y}}\|_2}{\left(\sum_{i=0}^2 |\hat{\lambda}|^i \|R_i\|_2\right) \|\hat{\mathbf{y}}\|_2}. \quad (7)$$

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

$$\eta(R, \hat{\lambda}, \hat{\mathbf{y}}) \geq \eta(R, \tilde{\lambda}, \tilde{\mathbf{y}}). \quad (8)$$

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

$$\eta(Q, \hat{\lambda}, V\hat{\mathbf{y}}) \geq \eta(Q, \tilde{\lambda}, V\tilde{\mathbf{y}}). \quad (9)$$

We will need the following lemma.

Lemma 1 *Let $(\hat{\lambda}, \hat{\mathbf{y}})$ be an approximate eigenpair of $R(\lambda)$ in (2) with $\hat{\mathbf{y}}$ normalized so that $\|\hat{\mathbf{y}}\|_2 = 1$. Then for the approximate eigenpair $(\hat{\lambda}, V\hat{\mathbf{y}})$ of $Q(\lambda)$ we have*

$$L_1(\hat{\lambda})\eta(R, \hat{\lambda}, \hat{\mathbf{y}}) \leq \eta(Q, \hat{\lambda}, V\hat{\mathbf{y}}) \leq L_2(\hat{\lambda}, \hat{\mathbf{y}})\eta(R, \hat{\lambda}, \hat{\mathbf{y}}),$$

where

$$L_1(\hat{\lambda}) := \frac{\left(\sum_{i=0}^2 |\hat{\lambda}|^i \|V^H A_i V\|_2\right)}{\left(\sum_{i=0}^2 |\hat{\lambda}|^i \|A_i\|_2\right)},$$

$$L_2(\hat{\lambda}, \hat{\mathbf{y}}) := \frac{\|Q(\hat{\lambda})V\hat{\mathbf{y}}\|_2}{\|R(\hat{\lambda})\hat{\mathbf{y}}\|_2}.$$

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

(QED)

Based on Lemma 1, we have the following theorem.

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

$$\kappa := \alpha \frac{L_1(\hat{\lambda})}{L_2(\tilde{\lambda}, \tilde{\mathbf{y}})} \geq 1 \quad (10)$$

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

Proof Based on Lemma 1, we have

$$\begin{aligned} \eta(Q, \hat{\lambda}, V\hat{\mathbf{y}}) &\geq L_1(\hat{\lambda})\eta(R, \hat{\lambda}, \hat{\mathbf{y}}) \\ &= L_1(\hat{\lambda}) \frac{\eta(R, \hat{\lambda}, \hat{\mathbf{y}})}{\eta(R, \tilde{\lambda}, \tilde{\mathbf{y}})} \eta(R, \tilde{\lambda}, \tilde{\mathbf{y}}) \\ &\geq \alpha \frac{L_1(\hat{\lambda})}{L_2(\tilde{\lambda}, \tilde{\mathbf{y}})} \eta(Q, \tilde{\lambda}, V\tilde{\mathbf{y}}) \\ &= \kappa \eta(Q, \tilde{\lambda}, V\tilde{\mathbf{y}}). \end{aligned}$$

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

(QED)

Let us examine the condition in (10). It is easy to show that $L_1(\hat{\lambda}) \leq 1$ and that $L_2(\tilde{\lambda}, \tilde{\mathbf{y}}) \geq 1$ so that

$L_1(\hat{\lambda})/L_2(\tilde{\lambda}, \tilde{\mathbf{y}}) \leq 1$. 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 $L_1(\hat{\lambda}) \approx 1$. Also, if the norm of the residual for the approximate eigenpair $(\tilde{\lambda}, \tilde{\mathbf{y}})$ of $R(\lambda)$ is small then we can expect the norm of the residual $Q(\tilde{\lambda})V\tilde{\mathbf{y}}$ to be small as well so that $L_2(\tilde{\lambda}, \tilde{\mathbf{y}}) \approx 1$. 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 NLEVP [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 Γ 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

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

$$\omega_p = \frac{(z_p - c)}{N}, \quad p = 1, \dots, N.$$

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 $\|V^H A_1 V\|_2^2 \leq \|V^H A_2 V\|_2 \|V^H A_0 V\|_2$. Hence, for these two problems, `quadeig` is called with the Fan, Lin and Van Dooren scaling γ_{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 γ_{trop}^+ (Table 4 shows that $\gamma_{trop}^+ \approx 10^3$ for both problems). With this choice of scalings, `quadeig` guarantees to return eigenpairs $(\tilde{\lambda}, \tilde{\mathbf{y}})$ inside Γ with backward errors $\eta(R, \tilde{\lambda}, \tilde{\mathbf{y}}) \lesssim nu$, where u is the machine precision. For these problems, `polyeig` returns eigenpairs $(\hat{\lambda}, \hat{\mathbf{y}})$ with $\eta(R, \hat{\lambda}, \hat{\mathbf{y}}) \gg nu$ so that (8) holds.

Table 4 displays the smallest value κ_{\min} of κ in (10), where $\hat{\lambda}$ corresponds to eigenvalues computed by `polyeig` and $(\tilde{\lambda}, \tilde{\mathbf{y}})$ are the corresponding eigenpairs computed by `quadeig`. Table 4 shows that the assump-

Table 1. List of test problems.

Problem	n	applications
damped_beam	400	vibration analysis
wiresaw2	500	vibration analysis of a wiresaw
mod_spring	200	damped mass-spring system
mod_sleeper	1000	oscillations of a rail track

Table 2. Parameters for the SS-RR method.

Problem	center c	radius r	#eigs
damped_beam	$-2 + 2.6 \times 10^6 i$	3×10^5	22
wiresaw2	$1.5 \times 10^3 i$	40	26
mod_spring	-5000	50	14
mod_sleeper	-1650	15	24

Table 3. Norm of the coefficient matrices of $R(\lambda) = V^H Q(\lambda) V$.

Problem	$\ V^H A_0 V\ _2$	$\ V^H A_1 V\ _2$	$\ V^H A_2 V\ _2$
damped_beam	10^{10}	2×10^{-1}	2×10^{-3}
wiresaw2	10^6	2×10^1	5×10^{-1}
mod_spring	25	5×10^3	1
mod_sleeper	13	2×10^3	1

Table 4. Minimum value of κ in (10), type of scaling γ used with `quadeig` and its value.

Problem	κ_{\min}	Parameter scaling	
		γ	value
damped_beam	1.4	γ_{FLV}	3×10^6
wiresaw2	1×10^3	γ_{FLV}	2×10^3
mod_spring	6×10^2	γ_{trop}^+	5×10^3
mod_sleeper	4×10^3	γ_{trop}^+	2×10^3

Table 5. Largest backward errors of eigenpairs.

Problem	SS-RR with		
	polyeig	quadeig	nu
damped_beam	3×10^{-9}	2×10^{-13}	9×10^{-14}
wiresaw2	6×10^{-11}	8×10^{-15}	1×10^{-13}
mod_spring	4×10^{-10}	2×10^{-15}	4×10^{-14}
mod_sleeper	2×10^{-10}	5×10^{-15}	2×10^{-13}

tion $\kappa > 1$ 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 `polyeig`. 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 $\eta(Q, \tilde{\lambda}, V\tilde{y}) \lesssim nu$, 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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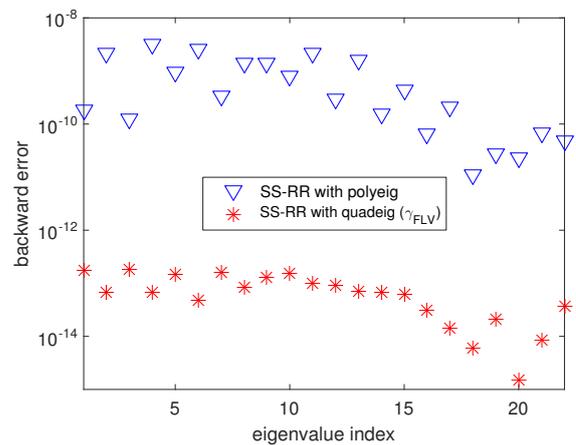


Fig. 1. Backward errors for the damped_beam problem.

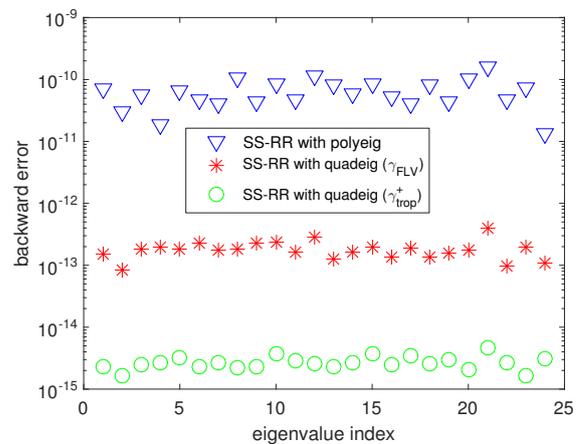


Fig. 2. Backward errors for the mod_sleeper problem.

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