DERIVATIVE INTERPOLATING SUBSPACE FRAMEWORKS FOR NONLINEAR EIGENVALUE PROBLEMS

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Abstract. We first consider the problem of approximating a few eigenvalues of a proper rational matrix-valued function closest to a prescribed target. It is assumed that the proper rational matrix-valued function is expressed in the transfer function form

$$H(s) = C(sI - A)^{-1}B,$$

where the middle factor is large, whereas the number of rows of $C$ and the number of columns of $B$ are equal and small. We propose a subspace framework that performs two-sided projections on the state-space representation of $H(\cdot)$, commonly employed in model reduction and giving rise to a reduced transfer function. At every iteration, the projection subspaces are expanded to attain Hermite interpolation conditions at the eigenvalues of the reduced transfer function closest to the target, which in turn leads to a new reduced transfer function. We prove in theory that, when a sequence of eigenvalues of the reduced transfer functions converges to an eigenvalue of the full problem, it converges at least at a quadratic rate. In the second part, we extend the proposed framework to locate the eigenvalues of a general square large-scale nonlinear meromorphic matrix-valued function $T(\cdot)$, where we exploit a representation $R(s) = C(s)A(s)^{-1}B(s) - D(s)$ defined in terms of the block components of $T(\cdot)$. The numerical experiments illustrate that the proposed framework is reliable in locating a few eigenvalues closest to the target point, and that, with respect to runtime, it is competitive to established methods for nonlinear eigenvalue problems.

Key words. Nonlinear eigenvalue problems, large scale, subspace projections, Hermite interpolation, quadratic convergence, rational eigenvalue problems.

AMS subject classifications. 65F15, 65D05, 34K17

1. Introduction. The numerical solutions of nonlinear eigenvalue problems have been a major field of research in the last twenty years [16, 10]. Numerical algorithms are proposed to estimate the eigenvalues of a nonlinear matrix-valued function either within a prescribed region, or closest to a prescribed target point in the complex plane.

Earlier works are mostly focused on polynomial and rational eigenvalue problems [20, 15, 19]. More recently, some of the attention has shifted to nonlinear eigenvalue problems that are neither polynomial nor rational. Various applications give rise to such non-polynomial, non-rational eigenvalue problems, including the stability analysis of delay systems [10], numerical solutions of elliptic PDE eigenvalue problems by the boundary element method [8], or finite element discretizations of differential equations with nonlinear boundary conditions depending on an eigenvalue parameter [6].

The nonlinear eigenvalue problem setting that we consider in this work is as follows. Let

$$(1.1) \quad T(s) := f_1(s)T_1 + \cdots + f_\kappa(s)T_\kappa,$$

where the functions $f_1, \ldots, f_\kappa : \mathbb{C} \to \mathbb{C}$ are meromorphic, and $T_1, \ldots, T_\kappa \in \mathbb{C}^{n \times n}$ are given matrices. Assume that the set $\{ \lambda \in \mathbb{C} \mid \text{rank}_{\lambda \in \mathbb{C}} T(\lambda) < n \}$ consists only of

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isolated points. Then we want to find $\lambda \in \mathbb{C}$ and $v \in \mathbb{C}^n \setminus \{0\}$ such that

(1.2) $T(\lambda)v = 0$.

The scalar $\lambda \in \mathbb{C}$ satisfying (1.2) is called an eigenvalue, and the vector $v \in \mathbb{C}^n \setminus \{0\}$ is called a corresponding eigenvector. This setting is quite general. For instance, polynomial and rational eigenvalue problems are special cases when $f_j(\cdot)$ are scalar-valued polynomials and rational functions, respectively. Delay eigenvalue problems can also be expressed in this form such that some of $f_j(\cdot)$ are exponential functions.

We propose an interpolation-based subspace framework to find a prescribed number of eigenvalues of $T(\cdot)$ closest to a given target point $\tau \in \mathbb{C}$. At every iteration, a projected small-scale nonlinear eigenvalue problem is solved. Then the projection subspaces are expanded so as to satisfy Hermite interpolation properties at the eigenvalues of the projected problem. The projections we rely on are devised from two-sided projections commonly employed in model-order reduction [5].

Our approach could be compared with linearization-based techniques for nonlinear eigenvalue problems. However, such techniques first use either polynomial interpolation [8] or rational interpolation [11] to approximate the nonlinear matrix-valued function with a polynomial or a rational matrix-valued function. Then the polynomial and rational eigenvalue problems are linearized into generalized eigenvalue problems. Finally, to deal with large-scale problems, typically Krylov subspace methods are applied to the generalized eigenvalue problem in an efficient manner, in particular taking the structure of the linearization into account; see for instance [21] and [14] for a one-sided and a two-sided rational Arnoldi method, respectively. The approach we propose here differs from these techniques, as it applies subspace projections directly to the nonlinear eigenvalue problem, and the projection subspaces are not necessarily Krylov subspaces. Consequently, our approach assumes the availability of numerical techniques for the solutions of the projected small-scale nonlinear eigenvalue problems. In the case of polynomial or rational eigenvalue problems, linearization-based techniques are available to our use to obtain all of the eigenvalues of the small-scale problem. Our numerical experience is that the proposed frameworks here are comparable to the state-of-the-art methods in terms of computational efficiency, and even a few times faster in some cases.

**Outline.** In the next section, we first describe an interpolatory subspace framework specifically for rational eigenvalue problems. For instance, for a proper rational matrix-valued function which can always be expressed in the form $R(s) = C(sI_k - A)^{-1}B$ for some $A \in \mathbb{C}^{k \times k}$, $B \in \mathbb{C}^{k \times m}$, and $C \in \mathbb{C}^{m \times k}$, the framework addresses the case when $k \gg m$ and reduces the dimension of the middle factor (i.e., it reduces the degrees of the numerators and denominators of the rational entries of the matrix-valued function). We give formal arguments establishing the quadratic convergence of the proposed subspace framework. In Section 3, we extend the subspace framework idea for rational eigenvalue problems to the general nonlinear eigenvalue problem setting of (1.2). Both Sections 2 and 3 present the frameworks to locate only one eigenvalue closest to the prescribed target. Section 4 discusses how they can be adapted to locate a prescribed number of closest eigenvalues to the target. Finally, Section 5 illustrates the frameworks on classical examples from the NLEVP data collection [6], and confirms the validity of the theoretical findings in practice.

**2. Rational Eigenvalue Problems.** A special important class of nonlinear eigenvalue problems are rational eigenvalue problems. There we want to find $\lambda \in \mathbb{C}$
and \( v \in \mathbb{C}^n \setminus \{0\} \) such that

\[
R(\lambda)v = 0, \quad \text{where} \quad R(s) := P(s) + \sum_{j=1}^\rho \frac{p_j(s)}{d_j(s)} E_j,
\]

and where \( d_j, p_j : \mathbb{C} \to \mathbb{C} \) are polynomials of degree \( k_j \) and strictly less than \( k_j \), respectively. Moreover, \( E_j \in \mathbb{C}^{n \times n} \) for \( j = 1, \ldots, \rho \) are given matrices, and \( P(\cdot) \) is a matrix polynomial of degree \( d \) of the form \( P(s) := s^d P_d + \cdots + s P_1 + P_0 \) for given \( P_0, \ldots, P_d \in \mathbb{C}^{n \times n} \). Again assume that the set \( \{ \lambda \in \mathbb{C} \mid \text{rank}_\mathbb{C} R(\lambda) < n \} \) consists only of isolated points.

The significance of the rational eigenvalue problem in (2.1) is due to several reasons. First, it is a cornerstone for the solutions of nonlinear eigenvalue problems that are not rational; such nonlinear eigenvalue problems are often approximated by rational eigenvalue problems. Secondly, there are several applications that give rise to rational eigenvalue problems such as models for vibrations of fluid-solid structure, as well as vibrating mechanical structures [16]. For instance, the latter leads to a rational eigenvalue problem involving the rational function

\[
R(s) = s^2M + K - \sum_{j=1}^\rho \frac{1}{1 + s\omega_j} G_j
\]

for symmetric mass and stiffness matrices \( M \) and \( K \), as well as the element stiffness matrices \( G_j \) and the relaxation parameters \( \omega_j \).

It is usually the case that the matrices \( E_j \) in (2.1) are of low rank, hence they can be decomposed into

\[
E_j = L_j U_j^*
\]

for some \( L_j, U_j \in \mathbb{C}^{n \times r_j} \) of full column rank such that \( r_j \ll n \). Additionally, the proper rational part of \( R(\cdot) \) can always be expressed as a transfer function associated with a linear time-invariant system. To this end, as argued in [3, page 95], we have

\[
\frac{p_j(s)}{d_j(s)} = a_j^*(sI_{k_j} - A_j)^{-1}b_j, \quad j = 1, \ldots, \rho
\]

for some \( A_j \in \mathbb{C}^{k_j \times k_j} \) and \( a_j, b_j \in \mathbb{C}^{k_j} \). Furthermore, using the low-rank decomposition (2.2), these transfer function representations can be combined into

\[
\sum_{j=1}^\rho \frac{p_j(s)}{d_j(s)} E_j = C(sI_k - A)^{-1}B, \quad \text{where}
\]

\[
A = \text{diag}(I_{r_1} \otimes A_1, \ldots, I_{r_\rho} \otimes A_\rho),
\]

\[
B = \begin{bmatrix} (I_{r_1} \otimes b_1)U_1^* \\ \vdots \\ (I_{r_\rho} \otimes b_\rho)U_\rho^* \end{bmatrix},
\]

\[
C = [L_1(I_{r_1} \otimes a_1)^* \ldots L_\rho(I_{r_\rho} \otimes a_\rho)^*],
\]

where \( \otimes \) denotes the Kronecker product and \( k := r_1k_1 + \cdots + r_\rho k_\rho \); see [19].

One way of dealing with (2.1) is to convert it into a generalized eigenvalue problem. For instance, for any \( k \times k \) matrix \( F \), we have

\[
C(\lambda F - A)^{-1}Bv = 0 \quad \Rightarrow \quad \begin{bmatrix} A & B \\ C & 0 \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \lambda F - A \end{bmatrix}^{-1}Bv = 0.
\]
More generally, \( \{ P(\lambda) + C(\lambda F - A)^{-1}B \} v = 0 \) for \( P(s) = \sum_{j=0}^{d} s^j P_j \) and for any \( k \times k \) matrix \( F \) can be linearized into

(2.5)

\[
(A - \lambda B)z = 0, \quad \text{where } z := \begin{bmatrix}
\lambda^{d-1}v \\
\lambda^{d-2}v \\
\vdots \\
v
\end{bmatrix},
\]

where we set \( d = 1 \) and \( P_0 = 0 \) in the case \( P(s) \equiv P_0 \). For \( F = I_n \), there is a one-to-one correspondence between the eigenvalues of \( \mathcal{L}(s) := A - sB \) and \( R(\cdot) \) as in (2.1). In particular, for this choice of \( F \) the following holds:

- If \( \lambda \) is an eigenvalue of the pencil \( \mathcal{L}(s) := A - sB \), but not an eigenvalue of \( A \), then \( \lambda \) is also an eigenvalue of \( R(\cdot) \) [19].
- Conversely, if \( \lambda \) is an eigenvalue of \( R(\cdot) \), it is also an eigenvalue of \( \mathcal{L}(\cdot) \); see also [18].

2.1. The Subspace Method for Rational Eigenvalue Problems. The setting we aim to address in this section is when the size of the matrix \( A \) as in (2.3) is very large compared to \( n \cdot d \), that is \( k \gg n \cdot d \), where \( k := r_1 k_1 + \cdots + r_\rho k_\rho \). Usually the ranks \( r_1, \ldots, r_\rho \) of \( E_1, \ldots, E_\rho \) are small, however it is possible that \( \rho \) is large (i.e., the proper rational part of \( R(\cdot) \) involves a weighted sum of many low rank matrices).

Here, we propose a subspace framework that replaces the proper rational part \( R_p(s) := C(sI - A)^{-1}B \) of \( R(\cdot) \) with a reduced one of the form

\[
R_p^{W,V}(s) := CV(sW^*V - W^*AV)^{-1}W^*B
\]

for two subspaces \( W, V \subseteq \mathbb{C}^k \) of equal dimension, say \( r \) such that \( r \ll k \), and matrices \( W, V \in \mathbb{C}^{k \times r} \) whose columns form orthonormal bases for the subspaces \( W, V \), respectively. We remark that the \( r \times r \) middle factor of the reduced proper rational function is much smaller than the \( k \times k \) middle factor of the full problem. The full rational function \( R_p(\cdot) \) and the reduced one \( R_p^{W,V}(\cdot) \) are the transfer functions of the linear time-invariant systems

(2.6)

\[
\frac{d}{dt}x(t) = Ax(t) + Bu(t), \quad y(t) = Cx(t)
\]

and

\[
\frac{d}{dt}W^*Vx(t) = W^*AVx(t) + W^*Bu(t), \quad y(t) = CVx(t),
\]

respectively. Hence, in the system setting, replacing \( R_p(\cdot) \) with \( R_p^{W,V}(\cdot) \) corresponds to restricting the state-space of (2.6) to \( V \), and then imposing a Petrov-Galerkin condition on the residual of the restricted state-space system to \( W \).

Our approach is interpolatory and inspired by model order reduction techniques [22, 7, 9, 4], as well as by a recent subspace framework proposed for the estimation of
the $\mathcal{H}_\infty$ norm of a transfer function $[1]$. The problem at hand (2.1) can be viewed as the minimization problem

$$\min_{\lambda \in \mathbb{C}} \sigma_{\min}(R(\lambda)).$$

Rather than this problem, at every iteration, we solve a reduced problem of the form

$$\min_{\lambda \in \mathbb{C}} \sigma_{\min}(R^{W,V}(\lambda)),$$

where $R^{W,V}(s) := P(s) + R_p^{W,V}(s)$. Then we expand the subspaces $W, V$ to $\tilde{W}, \tilde{V}$ so that

$$R(\tilde{\lambda}) = R^{\tilde{W},\tilde{V}}(\tilde{\lambda}) \quad \text{and} \quad R'(\tilde{\lambda}) = [R^{\tilde{W},\tilde{V}}]'(\tilde{\lambda})$$

at a global minimizer $\tilde{\lambda}$ of (2.7). The procedure is repeated by solving another reduced problem as in (2.7), but with $\tilde{W}, \tilde{V}$ taking the role of $W, V$.

One neat issue here is that finding the global minimizers of (2.7) amounts to computing the eigenvalues of the pencil

$$L^{W,V}(s) := [W^* 0 0 I_w] \begin{bmatrix} V & 0 \\ 0 & I_v \end{bmatrix} = A^{W,V} - sB^{W,V},$$

where

$$A^{W,V} := \begin{bmatrix} W^*AV & W^*B \\ CV & P_{d-1} \quad P_{d-2} \ldots \quad P_0 \\ -I_n & 0 \ldots & 0 \\ \cdots & \ddots & \vdots \\ -I_n & 0 \end{bmatrix},$$

$$B^{W,V} := \begin{bmatrix} W^*V \\ \vdots \\ -P_d \\ -I_n \\ \vdots \\ -I_n \end{bmatrix},$$

which is immediate from (2.5) by replacing $A, B, C, F$ with $W^*AV, W^*B, CV, W^*V$, respectively. We remark that the pencil $L^{W,V}(\cdot)$ in (2.9) is of size $(r + n \cdot d) \times (r + n \cdot d)$, whereas the original pencil $L(s) = A - sB$ is of size $(k + n \cdot d) \times (k + n \cdot d)$. As for the choice of at which eigenvalue $\lambda$ of $L^{W,V}(\cdot)$ we would Hermite interpolate, we prescribe a target $\tau$ a priori, and choose $\tilde{\lambda}$ as the eigenvalue of $L^{W,V}(\cdot)$ closest to $\tau$.

The only remaining issue that needs to be explained is how we expand the subspaces $W, V$ into $\tilde{W}, \tilde{V}$ so as to satisfy (2.8). Fortunately, the tools for this purpose have already been established as elaborated in the following result. This result is an immediate corollary of [5, Theorem 1].

**Lemma 2.1.** Suppose that $\mu \in \mathbb{C}$ is not an eigenvalue of $A$. Let $\tilde{W} = W \oplus W_\mu$ and $\tilde{V} = V \oplus V_\mu$, where $V, W$ are given subspaces of equal dimension, and $W_\mu, V_\mu$ are subspaces defined as

$$V_\mu := \bigoplus_{j=1}^q \text{Ran } ((A - \mu I)^{-j}B) \quad \text{and} \quad W_\mu := \bigoplus_{j=1}^q \text{Ran } ((C(A - \mu I)^{-j})^*)$$

for some positive integer $q$. Then we have
Algorithm 2.1 Subspace method to compute a rational eigenvalue closest to a prescribed target

Input: the matrices $P_1, \ldots, P_d \in \mathbb{C}^{n \times n}$ as in (2.1), and $A \in \mathbb{C}^{k \times k}$, $B \in \mathbb{C}^{k \times n}$, $C \in \mathbb{C}^{n \times k}$ as in (2.3), the interpolation parameter $q \in \mathbb{Z}$ with $q \geq 2$, the target $\tau \in \mathbb{C}$.

Output: the sequence $\{\lambda_\ell\}$ in $\mathbb{C}$.

1. $\lambda_1 \leftarrow \tau$.
2. for $\ell = 1, 2, \ldots$ do
   3. $\tilde{V}_\ell \leftarrow (A - \lambda_\ell I)^{-1}B$, $\tilde{W}_\ell \leftarrow (A - \lambda_\ell I)^{-*}C^*$, and $\tilde{W}_\ell \leftarrow \tilde{W}_\ell$.
   4. for $j = 2, \ldots, q$ do
      5. $\tilde{V}_\ell \leftarrow (A - \lambda_\ell I)^{-1}\tilde{W}_\ell$ and $\tilde{V}_\ell \leftarrow [\tilde{V}_\ell \; \tilde{V}_\ell]$.
      6. $\tilde{W}_\ell \leftarrow (A - \lambda_\ell I)^{-*}\tilde{W}_\ell$ and $\tilde{W}_\ell \leftarrow [\tilde{W}_\ell \; \tilde{W}_\ell]$.
   7. end for
   8. if $\ell = 1$ then
      9. $V_1 \leftarrow \text{orth} (\tilde{V}_1)$ and $W_1 \leftarrow \text{orth} (\tilde{W}_1)$.
   10. else
      11. $V_\ell \leftarrow \text{orth} \left( [V_{\ell-1} \; \tilde{V}_\ell] \right)$ and $W_\ell \leftarrow \text{orth} \left( [W_{\ell-1} \; \tilde{W}_\ell] \right)$.
   12. end if
   13. Form $L^{W_\ell,V_\ell}(s) \coloneqq A^{W_\ell,V_\ell} - sB^{W_\ell,V_\ell}$ as in (2.9).
   14. $\lambda_{\ell+1} \leftarrow$ the eigenvalue of $L^{W_\ell,V_\ell}(\cdot)$ closest to $\tau$.
   15. end for

1. $R(\mu) = R^{\tilde{W},\tilde{V}}(\mu)$, and
2. $R^{(j)}(\mu) = \left[ R^{\tilde{W},\tilde{V}} \right]^{(j)}(\mu)$ for $j = 1, \ldots, 2q - 1$,

where $R^{(j)}(\cdot)$ and $\left[ R^{\tilde{W},\tilde{V}} \right]^{(j)}(\cdot)$ denote the $j$th derivatives of $R(\cdot)$ and $R^{\tilde{W},\tilde{V}}(\cdot)$.

The resulting subspace method is described formally in Algorithm 2.1, where we assume that the proper rational part of $R(\cdot)$ is provided as an input in the transfer function form (2.3) in terms of $A$, $B$, $C$. At iteration $\ell$, the subspaces $V_{\ell-1}$, $W_{\ell-1}$ are expanded into $V_\ell$, $W_\ell$ in order to achieve $R(\Lambda_\ell) = R^{W_\ell,V_\ell}(\Lambda_\ell)$ as well as $R^{(j)}(\lambda_\ell) = \left[ R^{W_\ell,V_\ell} \right]^{(j)}(\lambda_\ell)$ for $j = 1, \ldots, 2q - 1$. Lines 3–12 of the algorithm fulfill this expansion task by augmenting $V_{\ell-1}$, $W_{\ell-1}$, matrices whose columns form orthonormal bases for $V_{\ell-1}$ and $W_{\ell-1}$, with additional columns as suggested by Theorem 2.1. Orthonormalizing the augmented matrices gives rise to the matrices $V_\ell$, $W_\ell$ whose columns span the expanded subspaces $V_\ell$, $W_\ell$, respectively. The next interpolation point $\lambda_{\ell+1}$ is then set equal to the eigenvalue of $L^{W_\ell,V_\ell}(\cdot)$ closest to the target point $\tau$.

The subsequent three subsections of this section establish the quadratic convergence of Algorithm 2.1. The arguments operate on the singular values of $R(s)$ and $R^{W_\ell,V_\ell}(s)$, especially their smallest singular values. Sections 2.2 and 2.3 focus on the interpolatory properties between these singular values, and the analytical properties of the singular values as a function of $s$. Finally, Section 2.4 deduces the main quadratic convergence result by exploiting these interpolatory and analytical properties.
2.2. Interpolation of Singular Values. Algorithm 2.1 is specifically tailored to satisfy the interpolation properties

\[(2.10) \quad R(\lambda_k) = R^{W_i,V_i}(\lambda_k) \quad \text{and} \quad R^{(j)}(\lambda_k) = \left[R^{W_i,V_i}\right]^{(j)}(\lambda_k)\]

for \(j = 1, \ldots, 2q - 1\) and \(k = 1, \ldots, \ell\). It is a simple exercise to extend this interpolation properties to the singular values of \(R(\lambda_k)\) and \(R^{W_i,V_i}(\lambda_k)\) for \(k = 1, \ldots, \ell\).

Formally, let us consider the eigenvalues of the matrices

\[M(s) := R(s)^*R(s) \quad \text{and} \quad M^{W_i,V_i}(s) := R^{W_i,V_i}(s)^*R^{W_i,V_i}(s)\]

as functions of \(s\) which we denote with \(\eta_1(s), \ldots, \eta_n(s)\) and \(\eta_1^{W_i,V_i}(s), \ldots, \eta_n^{W_i,V_i}(s)\) and which are sorted in descending order. These eigenvalues correspond to the squared singular values of the matrices \(R(s)\) and \(R^{W_i,V_i}(s)\), respectively. By the definitions of \(M(s)\) and \(M^{W_i,V_i}(s)\) and exploiting the interpolation properties \((2.10)\), next we deduce the desired interpolation result concerning the singular values. Throughout the rest of this section, we employ the notations

\[\eta'_j(s) := \begin{bmatrix} \frac{\partial \eta_j(s)}{\partial \Re(s)} & \frac{\partial \eta_j(s)}{\partial \Im(s)} \end{bmatrix} \quad \text{and} \quad \eta''_j^{W_i,V_i}(s) := \begin{bmatrix} \frac{\partial^2 \eta_j^{W_i,V_i}(s)}{\partial \Re(s)^2} & \frac{\partial^2 \eta_j^{W_i,V_i}(s)}{\partial \Re(s) \partial \Im(s)} & \frac{\partial^2 \eta_j^{W_i,V_i}(s)}{\partial \Im(s)^2} \end{bmatrix},\]

as well as

\[\nabla^2 \eta_j^{W_i,V_i}(s) := \begin{bmatrix} \frac{\partial^2 \eta_j^{W_i,V_i}(s)}{\partial \Re(s)^2} & \frac{\partial^2 \eta_j^{W_i,V_i}(s)}{\partial \Re(s) \partial \Im(s)} & \frac{\partial^2 \eta_j^{W_i,V_i}(s)}{\partial \Im(s)^2} \end{bmatrix}^{1/2}\]

for \(j = 1, \ldots, n\).

**Theorem 2.2** (Hermite interpolation). Regarding Algorithm 2.1 with \(q \geq 2\), the following assertions hold for \(k = 1, \ldots, \ell\) and \(j = 1, \ldots, n\):

(i) It holds that \(\eta_j(\lambda_k) = \eta_j^{W_i,V_i}(\lambda_k)\).

(ii) If \(\eta_j(\lambda_k)\) is simple, then also \(\eta_j^{W_i,V_i}(\lambda_k)\) is simple. In this case,

\[\eta'_j(\lambda_k) = \left[\eta''_j^{W_i,V_i}\right]'(\lambda_k) \quad \text{and} \quad \nabla^2 \eta_j(\lambda_k) = \nabla^2 \eta_j^{W_i,V_i}(\lambda_k).\]

**Proof.**

(i) The assertion immediately follows from \((2.10)\), since \(M(\lambda_k) = M^{W_i,V_i}(\lambda_k)\).

(ii) In Algorithm 2.1, it is required that \(q \geq 2\). Hence, the assertions follow from \((2.10)\), in particular from

\[M(\lambda_k) = M^{W_i,V_i}(\lambda_k),\]

\[M'(\lambda_k) = \left[M^{W_i,V_i}\right]'(\lambda_k),\]

\[M''(\lambda_k) = \left[M^{W_i,V_i}\right]''(\lambda_k),\]

by using the analytical formulas for the first and second derivatives of eigenvalue functions of a Hermitian matrix dependent on a real parameter [13].

The requirement that \(q \geq 2\) appears to be essential for quadratic convergence of the subspace framework. The arguments in the rest of this section establishing quadratic convergence does not apply for \(q = 1\). In practice, we observe slower convergence that is faster than linear convergence with \(q = 1\).
2.3. Analytical Properties of Singular Values. At an eigenvalue \( \lambda_\ast \) of \( R(\cdot) \), we must have \( \eta_\ast(\lambda_\ast) = 0 \). Additionally, throughout the rest of this section, the eigenvalue \( \lambda_\ast \) under consideration is assumed to be simple, i.e., \( \eta_1(\lambda_\ast), \ldots, \eta_{n-1}(\lambda_\ast) > 0 \). There are appealing smoothness properties intrinsic to \( \eta_1(\cdot), \ldots, \eta_n(\cdot) \) as well as \( \eta_{W_i, V_i}(\cdot) \) in a neighborhood of an eigenvalue \( \lambda_\ast \) of \( R(\cdot) \), as long as the following assumption holds.

**Assumption 2.3** (Non-defectiveness). Let \( \lambda_\ast \) be a simple eigenvalue of \( R(\cdot) \) such that, for a given \( \beta > 0 \), we have

\[
\sigma_{\min}(A - \lambda_\ast I_k) \geq \beta \quad \text{and} \quad \sigma_{\min}(W_\ell^* AV_\ell - \lambda_\ast W_\ell^* V_\ell) \geq \beta,
\]

where \( \sigma_{\min}(\cdot) \) denotes the smallest singular value of its matrix argument.

An implication of the assumption above, combined with the Lipschitz continuity of the singular value functions, is the boundedness of the smallest singular values in \( (2.11) \) away from zero in a vicinity of \( \lambda_\ast \). Formally, there exists a neighborhood \( N(\lambda_\ast) \) of \( \lambda_\ast \) independent of the choice of the subspaces \( V_\ell \) and \( W_\ell \) as long as \( (2.11) \) is satisfied – such that

\[
\sigma_{\min}(A - sI_k) \geq \beta/2 \quad \text{and} \quad \sigma_{\min}(W_\ell^* AV_\ell - sW_\ell^* V_\ell) \geq \beta/2 \quad \forall s \in N(\lambda_\ast),
\]

see the beginning of the proof of Lemma A.1 in [2].

The matrix-valued functions \( M(\cdot) \) and \( M^{W_\ell, V_\ell}(\cdot) \) are analytic in \( N(\lambda_\ast) \), which implies the following smoothness properties that we employ in the next section to analyze the rate of convergence. The proofs of the first three parts of the result below are straightforward adaptations of those for Lemma A.1 and Lemma A.2 in [2]. The proof of the fourth part is immediate from the second and third part. In the result and elsewhere, \( || \cdot ||_2 \) denotes the vector or matrix 2-norm. Moreover, we make use of the notation \( B(\lambda_\ast, \delta) \) for the open ball centered at \( \lambda_\ast \) with radius \( \delta > 0 \), that is

\[
B(\lambda_\ast, \delta) := \{ z \in \mathbb{C} \mid |z - \lambda_\ast| < \delta \},
\]

whereas \( \overline{B}(\lambda_\ast, \delta) \) denotes the closure of \( B(\lambda_\ast, \delta) \), that is the closed ball centered at \( \lambda_\ast \) with radius \( \delta > 0 \), i.e.,

\[
\overline{B}(\lambda_\ast, \delta) := \{ z \in \mathbb{C} \mid |z - \lambda_\ast| \leq \delta \}.
\]

By a constant here and in the subsequent arguments in this section, we mean that the scalar does not depend on \( \lambda_j \) for \( j = 1, \ldots, \ell \) as well as the subspaces \( W_\ell, V_\ell \). Rather, it can be expressed fully in terms of the quantities related to the original rational function \( R(\cdot) \).

**Lemma 2.4.** Suppose that Assumption 2.3 holds, and \( \lambda_\ell \) is sufficiently close to the eigenvalue \( \lambda_\ast \) of \( R(\cdot) \). There exist constants \( \gamma, \delta > 0 \) such that \( \overline{B}(\lambda_\ast, \delta) \subseteq N(\lambda_\ast) \) satisfying the following assertions:

(i) We have \( |\eta_j(s) - \eta_j(\hat{s})| \leq \gamma|s - \hat{s}| \) and \( |\eta_{W_\ell, V_\ell}^{j}(s) - \eta_{W_\ell, V_\ell}^{j}(\hat{s})| \leq \gamma|s - \hat{s}| \) for all \( s, \hat{s} \in B(\lambda_\ast, \delta) \) and for \( j = 1, \ldots, n \).

(ii) The eigenvalues \( \eta_n(s) \) and \( \eta_{W_\ell, V_\ell}^{n}(s) \) are simple for all \( s \in \overline{B}(\lambda_\ast, \delta) \). Hence, the derivatives

\[
\frac{\partial \eta_n(s)}{\partial s_1}, \frac{\partial^2 \eta_n(s)}{\partial s_1 \partial s_2}, \ldots, \frac{\partial^3 \eta_n(s)}{\partial s_1 \partial s_2 \partial s_3} \quad \text{and} \quad \frac{\partial \eta_{W_\ell, V_\ell}^{n}(s)}{\partial s_1}, \frac{\partial^2 \eta_{W_\ell, V_\ell}^{n}(s)}{\partial s_1 \partial s_2}, \ldots, \frac{\partial^3 \eta_{W_\ell, V_\ell}^{n}(s)}{\partial s_1 \partial s_2 \partial s_3}
\]

exist for every \( s_1, s_2, s_3 \in \{\text{Re}(s), \text{Im}(s)\} \) and for all \( s \in B(\lambda_\ast, \delta) \).
(iii) We have
\[
\left| \frac{\partial^2 \eta^{\ell_1, \ell_2}_{n_i}(s)}{\partial s_1} \right| \leq \gamma, \quad \left| \frac{\partial^2 \eta^{\ell_1, \ell_2}_{n_i}(s)}{\partial s_1 \partial s_2} \right| \leq \gamma, \quad \left| \frac{\partial^3 \eta^{\ell_1, \ell_2}_{n_i}(s)}{\partial s_1 \partial s_2 \partial s_3} \right| \leq \gamma
\]
for every \( s_1, s_2, s_3 \in \{\text{Re}(s), \text{Im}(s)\} \) and for all \( s \in B(\lambda_*, \delta) \).

(iv) We have
\[
\|\eta^{\ell_1}_n(s) - \hat{\eta}^{\ell_1}_n(\delta)\|_2 \leq \gamma|s - \delta|, \quad \left\| [\eta^{\ell_1, \ell_2}_n]'(s) - [\eta^{\ell_1, \ell_2}_n]'(\delta) \right\|_2 \leq \gamma|s - \delta|
\]
and
\[
\|\nabla^2 \eta^{\ell_1}_n(s) - \nabla^2 \eta^{\ell_1}_n(\delta)\|_2 \leq \gamma|s - \delta|, \quad \left\| \nabla^2 \eta^{\ell_1, \ell_2}_n(s) - \nabla^2 \eta^{\ell_1, \ell_2}_n(\delta) \right\|_2 \leq \gamma|s - \delta|
\]
for all \( s, \delta \in B(\lambda_*, \delta) \).

2.4. Convergence Properties. In practice, we observe that Algorithm 2.1 nearly always converges to the eigenvalue of \( R(\cdot) \) closest to the target point \( \tau \). Here, we consider two consecutive iterates \( \lambda_\ell, \lambda_{\ell+1} \) of this subspace method, which we assume close to an eigenvalue \( \lambda_* \) of \( R(\cdot) \). Then we prove
\[
|\lambda_{\ell+1} - \lambda_*| \leq C|\lambda_\ell - \lambda_*|^2
\]
for some constant \( C > 0 \). The closeness of \( \lambda_\ell, \lambda_{\ell+1} \) to \( \lambda_* \) is a silent assumption that is kept throughout, even though it is not explicitly stated. In addition, we deduce the bound (2.13) under Assumption 2.3, as well as the following assumption.

Assumption 2.5 (Non-degeneracy). The Hessian \( \nabla^2 \eta_n(\lambda_*) \) is invertible.

The main quadratic convergence result relies on the non-singularity of the Hessian of \( \eta^{\ell_1, \ell_2}_n(\cdot) \) in a ball centered around \( \lambda_* \). This is stated formally and proven next.

Lemma 2.6 (Uniform non-singularity of the Hessian). Suppose that Assumptions 2.3 and 2.5 hold. Then there exist constants \( \alpha, \delta > 0 \) such that
\[
\sigma_{\min}(\nabla^2 \eta^{\ell_1, \ell_2}_n(s)) \geq \alpha \quad \forall s \in B(\lambda_*, \delta).
\]

Proof. Let \( \beta := \sigma_{\min}(\nabla^2 \eta_n(\lambda_*)) > 0 \). By the Lipschitz continuity of \( \nabla^2 \eta_n(\cdot) \) around \( \lambda_* \) (which follows from part (iv) of Lemma 2.4), there exists a \( \hat{\delta} > 0 \) such that \( \sigma_{\min}(\nabla^2 \eta_n(s)) \geq \beta/2 \) for all \( s \in B(\lambda_*, \hat{\delta}) \). Without loss of generality, we may also assume that \( \nabla^2 \eta^{\ell_1, \ell_2}_n(\cdot) \) is Lipschitz continuous in \( B(\lambda_*, \hat{\delta}) \) with the Lipschitz constant \( \gamma \) (once again due to part (iv) of Lemma 2.4).

Setting \( \delta := \min \{\beta/(8\gamma), \hat{\delta}\} \), we additionally assume, without loss of generality, that \( \lambda_\ell \in B(\lambda_*, \delta) \). But then the Hermite interpolation property, specifically part (ii) of Theorem 2.2, implies
\[
\sigma_{\min}(\nabla^2 \eta^{\ell_1, \ell_2}_n(\lambda_\ell)) = \sigma_{\min}(\nabla^2 \eta_n(\lambda_\ell)) \geq \beta/2.
\]
Moreover,
\[
\left| \sigma_{\min}(\nabla^2 \eta^{\ell_1, \ell_2}_n(\lambda_\ell)) - \sigma_{\min}(\nabla^2 \eta^{\ell_1, \ell_2}_n(s)) \right| \leq \left\| \nabla^2 \eta^{\ell_1, \ell_2}_n(\lambda_\ell) - \nabla^2 \eta^{\ell_1, \ell_2}_n(s) \right\|_2 \leq \gamma|\lambda_\ell - s| \leq \beta/4
\]
for all \( s \in B(\lambda_*, \delta) \), where the first inequality follows from Weyl’s theorem [12, Theorem 4.3.1], whereas the second inequality is due to the Lipschitz continuity of \( \nabla^2 \eta^{\ell_1, \ell_2}_n(\cdot) \). Hence, we deduce \( \sigma_{\min}(\nabla^2 \eta^{\ell_1, \ell_2}_n(s)) \geq \beta/4 =: \alpha \) for all \( s \in B(\lambda_*, \delta) \) as desired. □
Now we are ready to present the main quadratic convergence result, where the notation $\mathcal{R}^2 : \mathbb{C} \to \mathbb{R}^2$ refers to the linear map defined by $\mathcal{R}^2(z) := [\text{Re}(z), \text{Im}(z)]$.

**Theorem 2.7** (Quadratic convergence). Suppose that Assumptions 2.3 and 2.5 hold. Then for the iterates of Algorithm 2.1 with $q \geq 2$, there exists a constant $C > 0$ such that (2.13) is satisfied.

**Proof.** Let $\delta$ be such that the assertions of Lemmas 2.4 and 2.6 hold in the ball $B(\lambda_*, \delta)$. In particular, the eigenvalues $\eta_n(\cdot)$ and $\eta_n^{W_i, V_i}(\cdot)$ are simple, $\nabla^2 \eta_n(\cdot)$ and $\nabla^2 \eta_n^{W_i, V_i}(\cdot)$ are Lipschitz continuous with Lipschitz constant $\gamma > 0$, and the lower bound (2.14) is satisfied for some constant $\alpha > 0$ in $B(\lambda_*, \delta)$. Without loss of generality, assume that $\lambda_{\ell+1}, \lambda_{\ell+1} \in B(\lambda_*, \delta)$.

The iterate $\lambda_{\ell+1}$, by definition, is an eigenvalue of $R^{W_i, V_i}(\cdot)$, hence we have $\eta_n^{W_i, V_i}(\lambda_{\ell+1}) = 0$. Indeed, $\lambda_{\ell+1}$ is a smooth global minimizer of $\eta_n^{W_i, V_i}(\cdot)$ (i.e., the smoothness follows from part (ii) of Lemma 2.4), implying also $\left[ \eta_n^{W_i, V_i} \right]^{\ell+1} = 0$.

By employing the Lipschitz continuity of $\nabla^2 \eta_n(\cdot)$ in $B(\lambda_*, \delta)$, we have

$$0 = \eta_n'(\lambda_\ell) = \eta_n'(\lambda_\ell) + \int_0^1 \nabla^2 \eta_n(\lambda_\ell + t(\lambda_* - \lambda_\ell)) \mathcal{R}^2(\lambda_* - \lambda_\ell) \, dt,$$

which, by exploiting $\nabla^2 \eta_n(\lambda_\ell) = \nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell)$ (see part (ii) of Theorem 2.2), could be arranged to

$$(2.15) \quad 0 = \eta_n'(\lambda_\ell) + \nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell) \mathcal{R}^2(\lambda_* - \lambda_\ell) + \int_0^1 (\nabla^2 \eta_n(\lambda_\ell + t(\lambda_* - \lambda_\ell)) - \nabla^2 \eta_n(\lambda_\ell)) \, \mathcal{R}^2(\lambda_* - \lambda_\ell) \, dt.$$ 

Moreover, by a Taylor expansion of $\eta_n^{W_i, V_i}(\cdot)$ about $\lambda_\ell$, we obtain

$$0 = \left[ \eta_n^{W_i, V_i} \right]'(\lambda_{\ell+1}) = \eta_n^{W_i, V_i}'(\lambda_\ell) + \nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell) \mathcal{R}^2(\lambda_{\ell+1} - \lambda_\ell) + \mathcal{O}(\|\lambda_{\ell+1} - \lambda_\ell\|^2),$$

which, combined with $\left[ \eta_n^{W_i, V_i} \right]'(\lambda_\ell) = \eta_n'(\lambda_\ell)$ (again due to part (ii) of Theorem 2.2), give rise to

$$(2.16) \quad \eta_n'(\lambda_\ell) + \nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell) \mathcal{R}^2(\lambda_* - \lambda_\ell) = \nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell) \mathcal{R}^2(\lambda_* - \lambda_{\ell+1}) + \mathcal{O}(\|\lambda_{\ell+1} - \lambda_\ell\|^2).$$

In (2.15), by plugging the right-hand side of (2.16), then exploiting the Lipschitz continuity of $\nabla^2 \eta_n(\cdot)$, and taking the norm, we deduce

$$(2.17) \quad \|\nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell) \mathcal{R}^2(\lambda_* - \lambda_{\ell+1})\|_2 \leq \frac{\gamma}{2} \|\lambda_* - \lambda_{\ell+1}\|^2 + \mathcal{O}(\|\lambda_{\ell+1} - \lambda_\ell\|^2),$$

where $\gamma$ is the Lipschitz constant for $\nabla^2 \eta_n(\cdot)$. Finally, by employing

$$\sigma_{\min}(\nabla^2 \eta_n^{W_i, V_i}(\lambda_\ell)) \geq \alpha$$

in (2.17) (which is implied by Lemma 2.6), we obtain

$$\alpha \|\lambda_{\ell+1} - \lambda_*\| \leq \frac{\gamma}{2} \|\lambda_* - \lambda_{\ell+1}\|^2 + \mathcal{O}(\|\lambda_{\ell+1} - \lambda_\ell\|^2).$$

The desired inequality (2.13) is now immediate from $\|\lambda_{\ell+1} - \lambda_\ell\| \leq 2 (\|\lambda_{\ell+1} - \lambda_*\|^2 + \|\lambda_* - \lambda_{\ell+1}\|^2)$. \qed
3. General Nonlinear Eigenvalue Problem Setting. Inspired by the ideas of the previous section for rational eigenvalue problems, we present a subspace framework for the more general setting of a nonlinear eigenvalue problem of the form (1.2). Let us consider $T(\cdot)$ and $T_j$ for $j = 1, \ldots, \kappa$ in (1.2) and (1.1) in the partitioned forms

$$
T(s) = \begin{bmatrix} A(s) & B(s) \\ C(s) & D(s) \end{bmatrix}
$$

and

$$
T_j = \begin{bmatrix} A_j & B_j \\ C_j & D_j \end{bmatrix},
$$

where $A(s), A_j \in \mathbb{C}^{k \times k}, B(s), B_j \in \mathbb{C}^{k \times m}, C(s), C_j \in \mathbb{C}^{m \times k}, D(s), D_j \in \mathbb{C}^{m \times m}$ for all $s \in \mathbb{C}$ such that $k + m = n$ and $k \gg m$. It is a simple exercise to deduce that every finite eigenvalue $\lambda \in \mathbb{C}$ of $T(\cdot)$ that is not an eigenvalue of $A(\cdot)$, is also an eigenvalue of the function

$$
\mathcal{R}(s) := C(s)A(s)^{-1}B(s) - D(s).
$$

Conversely, every finite eigenvalue of $\mathcal{R}(\cdot)$ is an eigenvalue of $T(\cdot)$.

Similar to the rational eigenvalue problem setting, the large-scale nature of $\mathcal{R}(\cdot)$ is hidden in the middle factor $A(\cdot)$. Hence, we define the reduced matrix-valued function corresponding to $\mathcal{R}(\cdot)$ by

$$
\mathcal{R}^{W,V}(s) := C(s)A^{W,V}(s)^{-1}B^{W}(s) - D(s)
$$

in terms of two subspaces $W, V \subseteq \mathbb{C}^r$ of equal dimension, say $r \ll k$, and matrices $W, V$ whose columns form orthonormal bases for them, where

$$
A^{W,V}(s) := W^*A(s)V = f_1(s)(W^*A_1V) + \cdots + f_\kappa(s)(W^*A_\kappa V),
$$

$$
B^{W}(s) := W^*B(s) = f_1(s)(W^*B_1) + \cdots + f_\kappa(s)(W^*B_\kappa),
$$

and

$$
C^{V}(s) := C(s)V = f_1(s)(C_1 V) + \cdots + f_\kappa(s)(C_\kappa V).
$$

The middle factor $A^{W,V}(\cdot)$ of the reduced matrix-valued function is of dimension $r \times r$ and much smaller than $A(\cdot)$.

Again, we benefit from the optimization point of view, that is we consider the minimization problem

$$
\min_{\lambda \in \mathbb{C}} \sigma_{\text{min}}(\mathcal{R}(\lambda)).
$$

In particular, assuming that the spectra of $A(\cdot)$ and $T(\cdot)$ are disjoint, the eigenvalue of $T(\cdot)$ closest to a prescribed target $\tau \in \mathbb{C}$ is the global minimizer of the optimization problem above closest to $\tau$. At every subspace iteration, instead of (3.3), we solve

$$
\min_{\lambda \in \mathbb{C}} \sigma_{\text{min}}(\mathcal{R}^{W,V}(\lambda)),
$$

specifically determine the global minimizer of $\mathcal{R}^{W,V}(\cdot)$ closest to the prescribed target $\tau$. The eigenvalues of $\mathcal{R}^{W,V}(\cdot)$ are the same as those of the function

$$
T^{W,V}(s) := \begin{bmatrix} A^{W,V}(s) & B^{W}(s) \\ C^{V}(s) & D(s) \end{bmatrix},
$$

except possibly those that are the eigenvalues of $A^{W,V}(\cdot)$. Hence, to retrieve the global minimizer $\tilde{\lambda}$ of $\sigma_{\text{min}}(\mathcal{R}^{W,V}(\cdot))$ closest to $\tau$, we find an eigenvalue of $T^{W,V}(\cdot)$ closest to this target point.
We expand the subspaces $W, V$ into $\tilde{W}, \tilde{V}$ so that

\begin{equation}
\mathcal{R}(\tilde{\lambda}) = \mathcal{R}^{\tilde{W}, \tilde{V}}(\tilde{\lambda}) \quad \text{and} \quad \mathcal{R}^{(j)}(\tilde{\lambda}) = \left[ \mathcal{R}^{\tilde{W}, \tilde{V}} \right]^{(j)}(\tilde{\lambda})
\end{equation}

hold for $j = 1, \ldots, q$ and for a prescribed positive integer $q$. The following generalization of Lemma 2.1 indicates how this Hermite interpolation property can be attained. This result is also a corollary of [5, Theorem 1].

**Lemma 3.1.** Suppose that $\mu \in \mathbb{C}$ is not an eigenvalue of $A(\cdot)$. Let $\tilde{W} = W \oplus W_\mu$ and $\tilde{V} = V \oplus V_\mu$, where $V, W$ are given subspaces of equal dimension, and $W_\mu, V_\mu$ are subspaces defined as

\begin{equation}
V_\mu := \bigoplus_{j=0}^{q-1} \text{Ran} \left( \frac{d^j}{ds^j} (A(s)^{-1}B(s)) \bigg|_{s=\mu} \right), \quad W_\mu := \bigoplus_{j=0}^{q-1} \text{Ran} \left( \frac{d^j}{ds^j} (C(s)A(s)^{-1})^* \bigg|_{s=\mu} \right)
\end{equation}

for some positive integer $q$. Then we have

1. $\mathcal{R}(\mu) = \mathcal{R}^{\tilde{W}, \tilde{V}}(\mu)$, and
2. $\mathcal{R}^{(j)}(\mu) = \left[ \mathcal{R}^{\tilde{W}, \tilde{V}} \right]^{(j)}(\mu)$ for $j = 1, \ldots, 2q - 1$.

Based on the discussions and the subspace expansion strategy above, we outline the subspace framework to locate the eigenvalue of $T(\lambda)$ closest to the target point $\tau \in \mathbb{C}$ in Algorithm 3.1. At iteration $\ell$ of the algorithm, first the subspaces $W_{\ell-1}, V_{\ell-1}$ are expanded to $W_{\ell}, V_{\ell}$ to achieve Hermite interpolation conditions at the current candidate $\lambda_\ell$ for the eigenvalue in lines 4–13. Then the next candidate $\lambda_{\ell+1}$ is retrieved by computing the eigenvalue of $T^{W_{\ell}, V_{\ell}}(\cdot)$ closest to the target point.

The quick convergence result of Theorem 2.7 extends to Algorithm 3.1 in a straightforward fashion. Specifically, two consecutive iterates $\lambda_\ell, \lambda_{\ell+1}$ of Algorithm 3.1 satisfy

$$|\lambda_{\ell+1} - \lambda_\star| \leq C|\lambda_\ell - \lambda_\star|^2$$

for some constant $C > 0$, provided $\lambda_\ell, \lambda_{\ell+1}$ are sufficiently close to an eigenvalue $\lambda_\star$ and under non-defectiveness and non-degeneracy assumptions analogous to Assumptions 2.3 and 2.5.

**4. Computing Multiple Eigenvalues.** The proposed subspace frameworks, Algorithms 2.1 and 3.1 for rational eigenvalue problems and general nonlinear eigenvalue problems, are meant to estimate only one eigenvalue closest to the prescribed target $\tau$. However, they have natural extensions to compute $k$ eigenvalues closest to the target for a prescribed integer $k \geq 2$. These extensions are based on extracting multiple eigenvalues of the projected problems, and expanding the projection spaces so as to ensure Hermite interpolation at some of these eigenvalues.

Before proposing three alternatives for the interpolation points, let us remark a subtle issue. There is the possibility that some of the eigenvalues of the projected problems $L^{W,V}(\cdot)$ and $T^{W,V}(\cdot)$ are indeed also the eigenvalues of their top-left blocks $L^{W,V}(s) := W^*AV - sW^*V$ and $A^{W,V}(\cdot)$. Even though this situation seems unlikely, we observe in practice that it sometimes occurs when multiple eigenvalues of the projected problems are extracted. We do not take such eigenvalues of $L^{W,V}(s)$ and $T^{W,V}(s)$ into consideration; such eigenvalues may correspond to the poles of $R^{W,V}(\cdot)$ and $\tilde{R}^{W,V}(\cdot)$ rather than the eigenvalues of $R^{W,V}(\cdot)$ and $\tilde{R}^{W,V}(\cdot)$.

To summarize, in lines 14 and 15 of Algorithms 2.1 and 3.1, we choose the interpolation points for the next iteration from the set $A^{W,V}(\cdot)$ consisting of all (finite) eigenvalues of $L^{W,V}(\cdot)$ and $T^{W,V}(\cdot)$ that are not eigenvalues of $L^{W,V}(\cdot)$ and $A^{W,V}(\cdot)$.
Algorithm 3.1 Subspace method to compute a nonlinear eigenvalue closest to a prescribed target

**Input:** the matrices $T_1, \ldots, T_k \in \mathbb{C}^{n \times n}$, the meromorphic functions $f_1, \ldots, f_k : \mathbb{C} \to \mathbb{C}$ as in (1.1), the partition parameter $m \in \mathbb{Z}^+$, the interpolation parameter $q \in \mathbb{Z}$ with $q \geq 2$, and the target point $\tau \in \mathbb{C}$.

**Output:** the sequence $\{\lambda_{\ell}\}$ in $\mathbb{C}$.

1. Partition $T(s)$ as in (3.1) so that $A(s) \in \mathbb{C}^{k \times k}$, $B(s) \in \mathbb{C}^{k \times m}$, $C(s) \in \mathbb{C}^{m \times k}$, $D(s) \in \mathbb{C}^{m \times m}$ for all $s \in \mathbb{C}$, where $k := n - m$.

2. $\lambda_1 \leftarrow \tau$.

3. for $\ell = 1, 2, \ldots$ do
   4. $\hat{V}_\ell \leftarrow A(\lambda_\ell) - B(\lambda_\ell)$ and $\hat{W}_\ell \leftarrow A(\lambda_\ell)^{-*}C(\lambda_\ell)^*$.
   5. for $j = 1, \ldots, q - 1$ do
      6. $\hat{V}_\ell \leftarrow \frac{d}{ds} (A(s)^{-1}B(s))|_{s=\lambda_\ell}$ and $\hat{V}_\ell \leftarrow \begin{bmatrix} \hat{V}_\ell & \hat{V}_\ell \end{bmatrix}$.
      7. $\hat{W}_\ell \leftarrow \frac{d}{ds} (A(s)^{-*}C(s)^*)|_{s=\lambda_\ell}$ and $\hat{W}_\ell \leftarrow \begin{bmatrix} \hat{W}_\ell & \hat{W}_\ell \end{bmatrix}$.
   end for
   9. if $\ell = 1$ then
   10. $V_1 \leftarrow \text{orth} \left( \hat{V}_1 \right)$ and $W_1 \leftarrow \text{orth} \left( \hat{W}_1 \right)$.
   else
   12. $V_\ell \leftarrow \text{orth} \left( \begin{bmatrix} V_{\ell-1} & \hat{V}_\ell \end{bmatrix} \right)$ and $W_\ell \leftarrow \text{orth} \left( \begin{bmatrix} W_{\ell-1} & \hat{W}_\ell \end{bmatrix} \right)$.
   end if
14. Form $T_{W_\ell, V_\ell}(s) := \begin{bmatrix} A_{W_\ell, V_\ell}(s) & B_{W_\ell}(s) \\ C_{V_\ell}(s) & D(s) \end{bmatrix}$, where $A_{W_\ell, V_\ell}()$, $B_{W_\ell}()$, $C_{V_\ell}()$ are defined as in (3.2).
15. $\lambda_{\ell+1} \leftarrow$ the eigenvalue of $T_{W_\ell, V_\ell}()$ closest to $\tau$.
16. end for

Specifically, we employ one of the following three viable strategies for the selection of the interpolation points at the next iteration among $\lambda_{\ell+1}^{(1)}, \ldots, \lambda_{\ell+1}^{(k)}$, the $k$ closest to the target point $\tau$ in $A_{W_\ell, V_\ell}$:

**NLALL:** Interpolate at up to all of the $k$ closest eigenvalues: Hermite interpolation is performed at the next iteration at each $\lambda_{\ell+1}^{(j)}$ unless the corresponding residual is below the convergence threshold for $j = 1, \ldots, k$.

**NLBR:** Interpolate at the eigenvalue among the $k$ closest with the best residual: Among the points $\lambda_{\ell+1}^{(1)}, \ldots, \lambda_{\ell+1}^{(k)}$ with residuals greater than the convergence threshold, we choose only the one with the smallest residual for Hermite interpolation at the next iteration.

**NLWR:** Interpolate at the eigenvalue among the $k$ closest with the worst residual: We perform Hermite interpolation at only one of $\lambda_{\ell+1}^{(1)}, \ldots, \lambda_{\ell+1}^{(k)}$, whichever has the largest residual.

5. Numerical Results. In this section, we apply the proposed subspace frameworks to several large-scale nonlinear eigenvalue problems. Our implementation and numerical experiments are performed in Matlab R2018a on an iMac with Mac OS 10.15.2 operating system, Intel® Core™ i5-9600K CPU and 32GB RAM.

The algorithms are terminated when the norms of the relative residuals of the Ritz pairs associated with the $k$ closest eigenvalues of the projected problems are less than the prescribed tolerance $\texttt{tol}$. Formally, letting $(\theta_j, v_j)$ denote the Ritz value
and vector associated with the \( j \)th closest eigenvalue of the projected problem for \( j = 1, \ldots, k \), we terminate if
\[
\text{Rs}(\theta_j, v_j) := \frac{\| T(\theta_j) v_j \|_\infty / \| v_j \|_\infty}{|f_1(\theta_j)| \| T_1 \|_\infty + \cdots + |f_m(\theta_j)| \| T_m \|_\infty} < \text{tol}
\]
for \( j = 1, \ldots, k \) for the general nonlinear eigenvalue problem setting of (1.2). A similar termination condition is adopted specifically for the rational eigenvalue problems. As termination tolerance we use \( \text{tol} = 10^{-12} \).

Some initializations and parameter values we employ are outlined next. We require the initial projected matrix \( A^{W_1, V_1}(\cdot) \) to be of size \( k \times k \) at least, where \( k \) is the prescribed number of closest eigenvalues to the target point. To make sure this is the case, we form the initial projected problem by interpolating the full problem at the target point, as well as at randomly selected points close to the target point unless otherwise specified. Throughout this section, we set the interpolation parameter \( q = 2 \) for Algorithms 2.1 and 3.1, and the partition parameter \( m = 2 \) for Algorithm 3.1.

The orthogonalization of the bases for the expansion subspaces (i.e., \( V_\ell, W_\ell \) in lines 11 and 12 of Algorithms 2.1 and 3.1) with respect to the existing projection subspaces (spanned by the columns of \( V_{\ell-1}, W_{\ell-1} \)) is performed several times in practice. This reorthogonalization strategy seems to improve the stability of the subspace frameworks, especially close to convergence.

In the subsequent three subsections, we present numerical results on rational eigenvalue problems, polynomial eigenvalue problems, and the gun problem, which is a nonlinear eigenvalue problem that is neither polynomial nor rational. In these subsections, when reporting the runtime, number of iterations, number of LU decompositions for a problem, we always run the algorithm five times, and present the average over the five runs.

### 5.1. Rational Eigenvalue Problems.

We first employ the variants of Algorithm 2.1 to locate several eigenvalues of a proper rational matrix-valued function \( R(s) = C(sI - A)^{-1}B \) closest to given target points, where \( A \in \mathbb{R}^{10^5 \times 10^5} \) is a sparse banded random matrix with bandwidth five, and \( B \in \mathbb{R}^{10^5 \times 2}, \ C \in \mathbb{R}^{2 \times 10^5} \) are also random matrices\(^1\). We perform experiments with two target points, namely \( \tau_1 = -2 + 3i \) and \( \tau_2 = 3 - 7i \); among these two, \( \tau_1 \) is close to the eigenvalues of \( R(\cdot) \), while \( \tau_2 \) is away from the eigenvalues of \( R(\cdot) \).

Our implementation to compute the eigenvalue of \( R(\cdot) \) closest to \( \tau_1 \) terminates with the estimate \(-2.000388770264 + 0.976430802383i\) after two subspace iterations. This estimate matches with the one returned by \texttt{eigs} (applied to a linearization as in (2.4)) up to all twelve decimal digits. However, the runtimes differ considerably, i.e., 0.55 seconds vs. 4.35 seconds in favor of Algorithm 2.1. The iterates \( \lambda_\ell \) of Algorithm 2.1 and the corresponding relative residuals are listed Table 5.1(a). The computation of the eigenvalue closest to \( \tau_2 \) requires additional iterations for the satisfaction of the termination condition. The computed eigenvalue after seven subspace iterations is \( 1.749889549609 - 3.144267920104i \), which is again the same as the estimate returned by \texttt{eigs} up to twelve decimal digits. Algorithm 2.1 takes a computation time of 1.90 seconds, while the runtime for \texttt{eigs} is 6.30 seconds. The last three estimates by Algorithm 2.1 and the corresponding residuals are given in Table 5.1(b).

Next we attempt to compute the five eigenvalues closest to the target points \( \tau_1 \) and \( \tau_2 \) by employing the variants \texttt{NLALL}, \texttt{NLBR}, and \texttt{NLWR} of Algorithm 2.1.

\(^1\)The precise matrices \( A, B, C \) for this proper rational eigenvalue problem are publicly available under the DOI 10.5281/zenodo.3902739.
Table 5.1

The iterates and the corresponding residuals of Algorithm 2.1 to locate the eigenvalue of the proper rational matrix-valued function closest to $\tau$.

(a) Results for $\tau_1 = -2 + i$.

<table>
<thead>
<tr>
<th>$\ell$</th>
<th>$\lambda_\ell$</th>
<th>$\text{Rs}(\lambda_\ell, v_\ell)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$-2.000383015796 + 0.976437330201$</td>
<td>$2.866 \cdot 10^{-7}$</td>
</tr>
<tr>
<td>2</td>
<td>$-2.000388770264 + 0.976430802383i$</td>
<td>$2.648 \cdot 10^{-16}$</td>
</tr>
</tbody>
</table>

(b) Results for $\tau_2 = 3 - 7i$.

<table>
<thead>
<tr>
<th>$\ell$</th>
<th>$\lambda_\ell$</th>
<th>$\text{Rs}(\lambda_\ell, v_\ell)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>$3.320019498487 - 2.968127299899i$</td>
<td>$1.077 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>6</td>
<td>$1.749889546050 - 3.144267907227i$</td>
<td>$1.330 \cdot 10^{-9}$</td>
</tr>
<tr>
<td>7</td>
<td>$1.749889549609 - 3.144267920104i$</td>
<td>$3.803 \cdot 10^{-19}$</td>
</tr>
</tbody>
</table>

All of these variants, as well as eigs return exactly the same five closest eigenvalues up to twelve decimal digits listed in Table 5.2. For the estimation of the five eigenvalues closest to $\tau_1$, the variants NLBR and NLWR need a runtime about 2.5–3 seconds while NLALL takes about 3–3.5 seconds and eigs takes about 5 seconds. There is a more significant difference in the runtimes to compute the eigenvalues closest to $\tau_2$, i.e., NLBR and NLWR take about 5.5–6 seconds, NLALL takes about 6.5–7 seconds, and eigs takes more than 16 seconds.

In the case of the computation of the five eigenvalues closest to $\tau_1$, in order to compare and illustrate the progresses of NLALL, NLWR, and NLBR, we present the relative residuals with respect to the number of iterations (until all five eigenvalues converge up to prescribed tolerance) in Table 5.3. The eigenvalue estimates corresponding to the residuals typed in blue italic letters are selected as interpolation points at the particular subspace iteration. Observe that the NLALL strategy interpolates at all five eigenvalue estimates in the first iteration, and four out of five eigenvalue estimates in the second iteration (as one eigenvalue has residual smaller than the prescribed tolerance in the second iteration, hence it is deemed to converge). In contrast, the NLBR and NLWR strategies interpolate at only one eigenvalue estimate at a given iteration. Specifically, NLBR interpolates at the eigenvalue with the smallest residual, whereas NLWR interpolates at the eigenvalue with the largest residual. In all of the tables, typically the relative residual of an eigenvalue estimate that is selected as an interpolation point decreases dramatically in the next iteration. A few exceptions to this are the three of the five interpolated eigenvalue estimates in the first iteration of NLALL, as well as the first two iterations of NLWR, where only modest reductions in the residuals are achieved possibly because the eigenvalue estimates are yet not close enough to the actual eigenvalues for the realization of the asymptotic quadratic rate of convergence.

Finally, we compare the performance of the three strategies and eigs to compute the $k$ closest eigenvalues for $k = 1, \ldots, 10$ to the target points $\tau_1$ and $\tau_2$. In Figures 5.1(a) and 5.1(b), the runtimes are plotted as a function of a prescribed number of closest eigenvalues for the target points $\tau_1$ and $\tau_2$, respectively. Even for $\tau_1$, the three variants NLALL, NLBR, and NLWR of Algorithm 2.1 are notably faster than eigs, though the gap in the runtimes closes as the prescribed number of eigenvalues increases. This difference in the runtimes of the three variants and eigs is more pronounced for the computation of $\tau_2$. The runtimes of NLALL, NLBR
Table 5.2
The computed kth closest eigenvalue $\lambda^{(k)}(\tau_j)$ for the proper rational matrix-valued function by Algorithm 2.1 to the target point $\tau_j$ for $k = 1, \ldots, 5$ and $j = 1, 2$, with $\tau_1 = -2 + i$ and $\tau_2 = 3 - 7i$.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$\lambda^{(1)}(\tau_1)$</th>
<th>$\lambda^{(1)}(\tau_2)$</th>
<th>$\lambda^{(2)}(\tau_1)$</th>
<th>$\lambda^{(2)}(\tau_2)$</th>
<th>$\lambda^{(3)}(\tau_1)$</th>
<th>$\lambda^{(3)}(\tau_2)$</th>
<th>$\lambda^{(4)}(\tau_1)$</th>
<th>$\lambda^{(4)}(\tau_2)$</th>
<th>$\lambda^{(5)}(\tau_1)$</th>
<th>$\lambda^{(5)}(\tau_2)$</th>
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<tbody>
<tr>
<td>1</td>
<td>1.749889549609</td>
<td>1.749889549609</td>
<td>2.046845106250</td>
<td>2.046845106250</td>
<td>2.90317282295</td>
<td>2.90317282295</td>
<td>2.90317282295</td>
<td>2.90317282295</td>
<td>2.90317282295</td>
<td>2.90317282295</td>
</tr>
<tr>
<td>2</td>
<td>1.501743427010</td>
<td>1.501743427010</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
<td>2.976251843638</td>
</tr>
<tr>
<td>3</td>
<td>1.338378173567</td>
<td>1.338378173567</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
<td>2.971362552627</td>
</tr>
<tr>
<td>4</td>
<td>1.801693244419</td>
<td>1.801693244419</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
<td>2.804111895782</td>
</tr>
</tbody>
</table>

Table 5.3
The residuals of the iters of the different variants of Algorithm 2.1 to compute the five eigenvalues of the proper rational matrix-valued function closest to $\tau_1 = -2 + i$. Interpolation is performed at the eigenvalue estimate whose residuals are typed in blue italic letters.

(a) Results for the variant NLALL.

<table>
<thead>
<tr>
<th>$\ell$</th>
<th>$\text{Rs}(\lambda^{(1)}_j, v^{(1)}_j)$</th>
<th>$\text{Rs}(\lambda^{(2)}_j, v^{(2)}_j)$</th>
<th>$\text{Rs}(\lambda^{(3)}_j, v^{(3)}_j)$</th>
<th>$\text{Rs}(\lambda^{(4)}_j, v^{(4)}_j)$</th>
<th>$\text{Rs}(\lambda^{(5)}_j, v^{(5)}_j)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.66·10^{-8}</td>
<td>2.86·10^{-6}</td>
<td>1.85·10^{-6}</td>
<td>9.95·10^{-7}</td>
<td>6.76·10^{-6}</td>
</tr>
<tr>
<td>2</td>
<td>2.42·10^{-19}</td>
<td>7.11·10^{-12}</td>
<td>1.44·10^{-8}</td>
<td>2.13·10^{-9}</td>
<td>3.48·10^{-8}</td>
</tr>
<tr>
<td>3</td>
<td>3.91·10^{-19}</td>
<td>2.48·10^{-18}</td>
<td>2.06·10^{-18}</td>
<td>9.08·10^{-19}</td>
<td>1.85·10^{-18}</td>
</tr>
</tbody>
</table>

(b) Results for the variant NLBR.

<table>
<thead>
<tr>
<th>$\ell$</th>
<th>$\text{Rs}(\lambda^{(1)}_j, v^{(1)}_j)$</th>
<th>$\text{Rs}(\lambda^{(2)}_j, v^{(2)}_j)$</th>
<th>$\text{Rs}(\lambda^{(3)}_j, v^{(3)}_j)$</th>
<th>$\text{Rs}(\lambda^{(4)}_j, v^{(4)}_j)$</th>
<th>$\text{Rs}(\lambda^{(5)}_j, v^{(5)}_j)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.56·10^{-10}</td>
<td>3.10·10^{-6}</td>
<td>4.11·10^{-6}</td>
<td>3.21·10^{-6}</td>
<td>1.65·10^{-6}</td>
</tr>
<tr>
<td>2</td>
<td>5.80·10^{-19}</td>
<td>4.40·10^{-7}</td>
<td>3.21·10^{-6}</td>
<td>1.08·10^{-6}</td>
<td>5.70·10^{-6}</td>
</tr>
<tr>
<td>3</td>
<td>1.45·10^{-18}</td>
<td>5.25·10^{-14}</td>
<td>5.46·10^{-6}</td>
<td>1.16·10^{-6}</td>
<td>5.89·10^{-6}</td>
</tr>
<tr>
<td>4</td>
<td>4.33·10^{-19}</td>
<td>2.04·10^{-15}</td>
<td>1.23·10^{-7}</td>
<td>9.23·10^{-13}</td>
<td>2.82·10^{-7}</td>
</tr>
<tr>
<td>5</td>
<td>2.83·10^{-19}</td>
<td>8.67·10^{-17}</td>
<td>9.51·10^{-19}</td>
<td>3.88·10^{-14}</td>
<td>9.41·10^{-10}</td>
</tr>
<tr>
<td>6</td>
<td>8.17·10^{-19}</td>
<td>9.08·10^{-18}</td>
<td>9.08·10^{-19}</td>
<td>3.10·10^{-15}</td>
<td>9.42·10^{-19}</td>
</tr>
</tbody>
</table>

(c) Results for the variant NLWR.

<table>
<thead>
<tr>
<th>$\ell$</th>
<th>$\text{Rs}(\lambda^{(1)}_j, v^{(1)}_j)$</th>
<th>$\text{Rs}(\lambda^{(2)}_j, v^{(2)}_j)$</th>
<th>$\text{Rs}(\lambda^{(3)}_j, v^{(3)}_j)$</th>
<th>$\text{Rs}(\lambda^{(4)}_j, v^{(4)}_j)$</th>
<th>$\text{Rs}(\lambda^{(5)}_j, v^{(5)}_j)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.54·10^{-9}</td>
<td>3.37·10^{-6}</td>
<td>4.83·10^{-6}</td>
<td>2.56·10^{-6}</td>
<td>4.32·10^{-6}</td>
</tr>
<tr>
<td>2</td>
<td>3.92·10^{-9}</td>
<td>7.58·10^{-6}</td>
<td>4.22·10^{-6}</td>
<td>4.26·10^{-6}</td>
<td>2.44·10^{-6}</td>
</tr>
<tr>
<td>3</td>
<td>5.58·10^{-10}</td>
<td>1.33·10^{-6}</td>
<td>3.64·10^{-6}</td>
<td>2.21·10^{-6}</td>
<td>4.77·10^{-6}</td>
</tr>
<tr>
<td>4</td>
<td>4.03·10^{-11}</td>
<td>7.34·10^{-8}</td>
<td>1.22·10^{-8}</td>
<td>7.31·10^{-8}</td>
<td>5.20·10^{-11}</td>
</tr>
<tr>
<td>5</td>
<td>2.77·10^{-12}</td>
<td>1.08·10^{-18}</td>
<td>1.56·10^{-9}</td>
<td>1.95·10^{-8}</td>
<td>1.04·10^{-11}</td>
</tr>
<tr>
<td>6</td>
<td>6.65·10^{-13}</td>
<td>1.18·10^{-18}</td>
<td>7.95·10^{-11}</td>
<td>7.21·10^{-19}</td>
<td>5.75·10^{-13}</td>
</tr>
<tr>
<td>7</td>
<td>2.60·10^{-14}</td>
<td>2.42·10^{-18}</td>
<td>1.21·10^{-18}</td>
<td>5.77·10^{-19}</td>
<td>1.51·10^{-15}</td>
</tr>
</tbody>
</table>

and NLWR are largely determined by the number of LU decompositions, as well as the number of forward and backward substitutions performed. Since the number of backward and forward substitutions is $n \cdot q$ times the number of LU decompositions in general, and specifically four (as $n = q = 2$) times the number of LU decompositions in all of these examples, we report only the number of LU decompositions as a function of the prescribed number of closest eigenvalues in Figures 5.1(c) and 5.1(d). The runtimes of NLALL, NLBR, and NLWR with the target point $\tau_1$ are similar as these three strategies require similar number of LU decompositions. On the
The residuals of the eigenvalue estimates of Algorithm 3.1 equipped with the NLALL strategy on the Schrödinger example and to compute the ten eigenvalues closest to \( \tau = -0.36 - 0.001i \) are given in Table 5.4.

<table>
<thead>
<tr>
<th>( \ell )</th>
<th>( \text{Rs} (\lambda_1^{(1)}, v_1^{(1)}) )</th>
<th>( \text{Rs} (\lambda_2^{(2)}, v_2^{(2)}) )</th>
<th>( \text{Rs} (\lambda_3^{(3)}, v_3^{(3)}) )</th>
<th>( \text{Rs} (\lambda_4^{(4)}, v_4^{(4)}) )</th>
<th>( \text{Rs} (\lambda_5^{(5)}, v_5^{(5)}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 1.05 \cdot 10^{-6} )</td>
<td>( 1.08 \cdot 10^{-8} )</td>
<td>( 1.64 \cdot 10^{-8} )</td>
<td>( 1.77 \cdot 10^{-8} )</td>
<td>( 3.02 \cdot 10^{-8} )</td>
</tr>
<tr>
<td>2</td>
<td>( 8.71 \cdot 10^{-16} )</td>
<td>( 9.37 \cdot 10^{-16} )</td>
<td>( 2.08 \cdot 10^{-15} )</td>
<td>( 5.70 \cdot 10^{-16} )</td>
<td>( 1.93 \cdot 10^{-15} )</td>
</tr>
<tr>
<td>( \ell )</td>
<td>( \text{Rs} (\lambda_6^{(6)}, v_6^{(6)}) )</td>
<td>( \text{Rs} (\lambda_7^{(7)}, v_7^{(7)}) )</td>
<td>( \text{Rs} (\lambda_8^{(8)}, v_8^{(8)}) )</td>
<td>( \text{Rs} (\lambda_9^{(9)}, v_9^{(9)}) )</td>
<td>( \text{Rs} (\lambda_{10}^{(10)}, v_{10}^{(10)}) )</td>
</tr>
<tr>
<td>1</td>
<td>( 1.26 \cdot 10^{-8} )</td>
<td>( 4.32 \cdot 10^{-8} )</td>
<td>( 2.68 \cdot 10^{-8} )</td>
<td>( 1.38 \cdot 10^{-8} )</td>
<td>( 5.88 \cdot 10^{-8} )</td>
</tr>
<tr>
<td>2</td>
<td>( 2.34 \cdot 10^{-15} )</td>
<td>( 2.83 \cdot 10^{-15} )</td>
<td>( 4.38 \cdot 10^{-15} )</td>
<td>( 1.34 \cdot 10^{-15} )</td>
<td>( 2.59 \cdot 10^{-15} )</td>
</tr>
</tbody>
</table>

5.2. Polynomial Eigenvalue Problems. Next we consider two large-scale polynomial eigenvalue problems available in the NLEVP collection [6]. Both of these involve quadratic matrix polynomials of the form \( P(s) = P_0 + sP_1 + s^2P_2 \) for given square matrices \( P_0, P_1, P_2 \in \mathbb{C}^{n \times n} \). The first one is the Schrödinger example with \( n = 1998 \) that arises from a discretization of the Schrödinger operator. We compute the \( k \) closest eigenvalues to the target point \( \tau = -0.36 - 0.001i \) for \( k = 1, \ldots, 10 \) using the variants NLALL, NLBR, and NLWR of Algorithm 3.1, as well as the latest version of a free Matlab implementation\(^2\) of the CORK algorithm [21]. In all cases, the computed eigenvalues by all these methods match exactly up to at least eight decimal digits. In particular, in Figure 5.2(a) the eigenvalues near the target point (computed by applying \text{eigs} to a linearization of \( P(\cdot) \)) are displayed with red crosses, and the ten closest eigenvalues computed by these methods are encircled in blue. In Figure 5.2(b), the runtimes in seconds for the three variants of Algorithm 3.1 and the CORK algorithm are plotted as a function of the prescribed number of eigenvalues. The runtimes appear to be similar, though the variants NLALL, NLWR look slightly faster. Computing these eigenvalues using \text{eigs} applied to a standard companion linearization of \( P(\cdot) \) results in precisely the same eigenvalues up to eight decimal digits, however the runtimes for \text{eigs} are much longer varying from 2.7 seconds to 4 seconds depending on the number of desired eigenvalues. For the NLALL variant of Algorithm 3.1 and to compute the ten eigenvalues closest to \( \tau \), the termination criterion is satisfied after two iterations. The residuals for the ten eigenvalue estimates at each of these two iterations are given in Table 5.4. Interpolation is performed at every one of the ten eigenvalue estimates at the first iteration. As a result, all residuals decrease dramatically in the next iteration.

The runtimes in seconds (top row), overall number of LU decompositions performed until termination (middle row), number of subspace iterations (bottom row) are shown as functions of prescribed number of eigenvalues for the variants of Algorithm 2.1 with the target points $\tau_1 = -2 + i$ on the left, $\tau_2 = 3 - 7i$ on the right.

(a) Runtime vs. number of eigenvalues for the target $\tau_1 = -2 + i$.

(b) Runtime vs. number of eigenvalues for the target $\tau_2 = 3 - 7i$.

(c) Number of LU decompositions vs. number of eigenvalues for the target $\tau_1 = -2 + i$.

(d) Number of LU decompositions vs. number of eigenvalues for the target $\tau_2 = 3 - 7i$.

(e) Number of iterations vs. number of eigenvalues for the target $\tau_1 = -2 + i$.

(f) Number of iterations vs. number of eigenvalues for the target $\tau_2 = 3 - 7i$.

Fig. 5.1. The runtimes in seconds (top row), overall number of LU decompositions performed until termination (middle row), number of subspace iterations (bottom row) are shown as functions of prescribed number of eigenvalues for the variants of Algorithm 2.1 with the target points $\tau_1 = -2 + i$ on the left, $\tau_2 = 3 - 7i$ on the right.
The second polynomial eigenvalue problem from the NLEVP collection is the \texttt{acoustic\_wave\_2d} example with $n = 100172$ that originates from a finite element discretization of the 2-dimensional acoustic wave equation. Once again, we estimate the $k$ closest eigenvalues for $k = 1, \ldots, 10$ to two target points, specifically to $\tau_1 = 4+0.1i$ and $\tau_2 = 2+3i$, by employing the variants \texttt{NLALL}, \texttt{NLBR}, and \texttt{NLWR} of Algorithm 3.1, and the \texttt{CORK} algorithm. The eigenvalues of the quadratic matrix polynomial that are close to these two target points are displayed in Figure 5.3 with red crosses. For each one of the two target points, all of the methods return exactly the same ten closest eigenvalues up to at least ten decimal digits. In Figure 5.3, the ten computed eigenvalues closest to $\tau_1$ are indicated with blue circles, whereas the ones closest to $\tau_2$ are depicted with blue diamonds. The first target point is in the interior of the spectrum, whereas the second one is far away. The convergence behaviors of the algorithms, as a result their runtimes, seem to be affected by the closeness of the target point to the spectrum. For the interior target point $\tau_1$, the \texttt{CORK} algorithm appears to be the fastest in locating the eigenvalues as illustrated in Figure 5.4(a). In contrast to that, for the exterior target point $\tau_2$, all three variants of Algorithm 3.1 appear to be faster than \texttt{CORK} as shown in Figure 5.4(b). In some of our trials (with default parameter values) with the exterior target point $\tau_2$, \texttt{CORK} also had convergence issues, e.g., it could not converge to all of the $k$ closest eigenvalues for $k = 6, 7, 8$, but the ones converged in these cases were among the $k$ closest.

We have tested the variants of Algorithm 3.1 with all of the large-scale quadratic eigenvalue problems in the NLEVP collection and compared them with the \texttt{CORK} algorithm. Our observation is that their runtimes are comparable (i.e., the runtimes differ by a few times at most in favor of one of the variants of Algorithm 3.1 or the \texttt{CORK} algorithm) when only a small number of closest eigenvalues to the target point are sought. In these limited experiments, the \texttt{NLALL} variant of Algorithm 3.1
appears to be the most reliable (among the three variants and the CORK algorithm with default parameter settings) in converging to the closest eigenvalues accurately.

5.3. The Gun Problem. The gun problem, originating from modeling of a radio-frequency gun cavity, concerns the solution of a nonlinear eigenvalue problem

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5_3.png}
\caption{The computed ten closest eigenvalues to $\tau_1 = 4 + 0.1i$ and $\tau_2 = 2 + 3i$ by Algorithm 3.1 for the \texttt{acoustic\_wave\_2d} example are illustrated with blue circles and diamonds, respectively. The red crosses and black asterisk mark the eigenvalues and $\tau_1 = 4 + 0.1i$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5_4.png}
\caption{The runtimes in seconds of the variants of Algorithm 3.1 and the CORK algorithm to compute the $k \in [1, 10]$ eigenvalues closest to a specified target for the \texttt{acoustic\_wave\_2d} example.}
\end{figure}
The residuals of the eigenvalue estimates of Algorithm 3.1 equipped with the NLALL strategy on the gun example to compute the five closest eigenvalues to \( \tau = (8 + 2.5i) \cdot 10^4 \).  

<table>
<thead>
<tr>
<th>( f )</th>
<th>( \text{Rs} \left( \lambda^{(1)}_f, v_f^{(1)} \right) )</th>
<th>( \text{Rs} \left( \lambda^{(2)}_f, v_f^{(2)} \right) )</th>
<th>( \text{Rs} \left( \lambda^{(3)}_f, v_f^{(3)} \right) )</th>
<th>( \text{Rs} \left( \lambda^{(4)}_f, v_f^{(4)} \right) )</th>
<th>( \text{Rs} \left( \lambda^{(5)}_f, v_f^{(5)} \right) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 8.43 \cdot 10^{-6} )</td>
<td>( 6.24 \cdot 10^{-4} )</td>
<td>( 1.03 \cdot 10^{-3} )</td>
<td>( 4.89 \cdot 10^{-4} )</td>
<td>( 2.86 \cdot 10^{-4} )</td>
</tr>
<tr>
<td>2</td>
<td>( 4.66 \cdot 10^{-7} )</td>
<td>( 4.19 \cdot 10^{-17} )</td>
<td>( 4.40 \cdot 10^{-9} )</td>
<td>( 3.81 \cdot 10^{-14} )</td>
<td>( 2.15 \cdot 10^{-11} )</td>
</tr>
<tr>
<td>3</td>
<td>( 1.70 \cdot 10^{-17} )</td>
<td>( 2.86 \cdot 10^{-17} )</td>
<td>( 1.42 \cdot 10^{-17} )</td>
<td>( 4.23 \cdot 10^{-17} )</td>
<td>( 2.03 \cdot 10^{-17} )</td>
</tr>
</tbody>
</table>

The residuals of the eigenvalue estimates of Algorithm 3.1 equipped with the NLALL strategy on the gun example to compute the five closest eigenvalues to \( \tau = (8 + 2.5i) \cdot 10^4 \) for \( k = 1, \ldots, 10 \) inside the specified upper half-disk by employing the NLALL variant of Algorithm 3.1. The eigenvalues of the reduced problems are computed using the Matlab implementation of NLEIGS [11] that is available on the internet\(^3\). The initial interpolation points are not chosen randomly anymore. Rather, in addition to the target point \( \tau \), we employ the following eight interpolation points initially: 

|\( P_0 \cdot \lambda P_1 + i\sqrt{\lambda - \sigma_1^2 W_1} + i\sqrt{\lambda - \sigma_2^2 W_2} \) \( v \) = 0 |

for given real symmetric matrices \( P_0, P_1, W_1, W_2 \in \mathbb{R}^{9956 \times 9956} \) with positive semidefinite \( P_0 \) and positive definite \( P_1 \). With the parameters \( \sigma_1 = 0 \) and \( \sigma_2 = 108.8774 \), the eigenvalues inside the upper half-disk in the complex plane centered at \( 250^2 \) and with radius \( 300^2 - 250^2 \) are reported in several works in the literature.

Here, we compute the \( k \) eigenvalues closest to the target \( \tau = (8 + 2.5i) \cdot 10^4 \) for \( k = 1, \ldots, 10 \) inside the specified upper half-disk by employing the NLALL variant of Algorithm 3.1. The eigenvalues of the reduced problems are computed using the Matlab implementation of NLEIGS [11] that is available on the internet\(^3\). The initial interpolation points are not chosen randomly anymore. Rather, in addition to the target point \( \tau \), we employ the following eight interpolation points initially: 

\[ 3 \cdot 10^3, 9 \cdot 10^3, (2+i) \cdot 10^3, (6+i) \cdot 10^3, (10+i) \cdot 10^3, (2+3i) \cdot 10^3, (6+3i) \cdot 10^3, (10+3i) \cdot 10^3. \]

The computed five closest eigenvalues (encircled in blue) together with all eigenvalues (marked with red crosses) inside the half-disk are shown in Figure 5.5(a). In all cases, the computed eigenvalues are the same as those returned by NLEIGS applied directly to the full problem at least up to nine decimal digits. However, the direct application of NLEIGS takes about 38 seconds of computation time, whereas the NLALL variant requires considerably less computing time; see the runtimes for the NLALL variant in Figure 5.5(b). The runtime of the NLALL variant is once again mainly affected by the number of LU decompositions (which is also displayed in Figure 5.5(b)), as well as the number of forward and backward substitutions performed (which is four times the number of LU decompositions in each case).

The progress of the algorithm to compute the five eigenvalues closest to the target point can be observed in Table 5.5, where the residuals are given at every iteration up until the satisfaction of the termination criterion. Once again, the residual for an eigenvalue estimate usually decays considerably when Hermite interpolation is performed at that eigenvalue estimate.

### 6. Concluding Remarks

We have proposed subspace frameworks based on Hermite interpolation to deal with the estimation of a few eigenvalues of a large-scale nonlinear matrix-valued function closest to a prescribed target. At every subspace iteration, first a reduced nonlinear eigenvalue problem is obtained by employing two-sided projections inspired from interpolatory model-order reduction techniques, then the eigenvalues of the reduced eigenvalue problem are extracted, and finally the projection subspaces are expanded to attain Hermite interpolation between the full and reduced problem at the eigenvalues of the reduced problem. We have proven that

\(^3\)available at http://twr.cs.kuleuven.be/research/software/nleps/nleigs.html
the proposed framework converges at least at a quadratic rate in theory under a non-defectiveness and a non-degeneracy assumption.

The proposed framework appears to be usually reliable in locating a prescribed number of closest eigenvalues accurately, especially when interpolation is enforced at every eigenvalue of the reduced problem close to the target point. Such a strategy seems to be also comparable to the best existing methods in terms of runtime. An alternative is to interpolate at only one eigenvalue of the reduced problem at every subspace iteration.

There are several directions that are open to improvement. One of them is the initial selection of the interpolation points. This may affect the number of subspace iterations. At the moment, we choose the initial interpolation points randomly around the target. A more careful selection of them, for instance using the AAA algorithm [17], may reduce the number of subspace iterations. Another issue is the partitioning of the nonlinear matrix-valued function $T(\cdot)$ as in (3.1), where $B(\cdot)$ has few columns and $C(\cdot)$ has few rows. This partitioning may affect the convergence and stability properties of the framework. It seems even possible to permute the rows and columns of $T(\cdot)$, and more generally apply unitary transformations from left or right in advance with the purpose of enhancing the convergence and stability properties. We hope to address these issues in a future work.

Software. Matlab implementations of NLALL, NLBR, NLWR variants of Algorithms 2.1 and 3.1, and the rational eigenvalue problem example that is experimented on in Section 5.1 are publicly available under the DOI 10.5281/zenodo.3902739. All other nonlinear eigenvalue problem examples on which we perform numerical experiments in Section 5 are also publicly available in the NLEVP collection [6].
REFERENCES


