Several properties of invariant pairs of nonlinear algebraic eigenvalue problems

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SEVERAL PROPERTIES OF INVARIANT PAIRS OF NONLINEAR ALGEBRAIC EIGENVALUE PROBLEMS*

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Abstract. We analyze several important properties of invariant pairs of nonlinear algebraic eigenvalue problems of the form $T(\lambda)v = 0$. Invariant pairs are generalizations of invariant subspaces in association with block Rayleigh quotients of square matrices to a nonlinear matrix-valued function $T(\cdot)$. They play an important role in the analysis of nonlinear eigenvalue problems and algorithms. In this paper, we first show that the algebraic, partial, and geometric multiplicities together with the Jordan chains corresponding to an eigenvalue of $T(\lambda)v = 0$ are completely represented by the Jordan canonical form of a simple invariant pair that captures this eigenvalue. We then investigate approximation errors and perturbations of a simple invariant pair. We also show that second order accuracy in eigenvalue approximation can be achieved by the two-sided block Rayleigh functional for non-defective eigenvalues. Finally, we study the matrix representation of the Fréchet derivative of the eigenproblem, and we discuss the norm estimate of the inverse derivative, which measures the conditioning and sensitivity of simple invariant pairs.

Key words. nonlinear eigenvalue problems, Jordan chains, invariant pairs, approximation error, perturbation analysis, Rayleigh functional, Newton-Kantorovich theorem

AMS subject classifications. 65F15, 65F10, 65F50, 15A18, 15A22.

1. Introduction.

The development of theory and numerical methods for nonlinear algebraic eigenvalue problems has attracted considerable attention in recent years. These problems arise from a large variety of applications, such as dynamic analysis of structures, study of singularities in elastic materials, optimization of the acoustic emissions of high speed trains, and minimization of the cost functional for optimal control problems; see, e.g., [1], [16], [17], [31]. Polynomial and rational eigenvalue problems, and especially quadratic problems, are of particular interest. These problems can be equivalently transformed to a linear eigenvalue problem of larger size by some appropriate form of linearizations; see, e.g., [13], [14], [29]. Nonlinear eigenvalue problems are generally much more challenging than their linear counterparts. For example, these problems are highly structured in many cases, and the structure often needs to be taken into full account for the development of analysis and algorithms; in addition, deflation of converged eigenpairs is not straightforward, because eigenvectors corresponding to distinct eigenvalues can be linearly dependent.

This paper concerns the study of several important algebraic and analytical properties of invariant pairs for general nonlinear algebraic eigenvalue problems of the form $T(\lambda)v = 0$. Invariant pairs, introduced by Kressner [12], are generalizations of invariant subspaces and associated subspace projections of square matrices. The computation of invariant pairs are considered a practical and effective approach to provide approximations to a set of eigenpairs simultaneously, especially for degenerate (semi-simple or defective) eigenvalues, or eigenpairs with linearly dependent eigenvectors. In particular, a block version of Newton's method studied in [12] is shown to exhibit locally quadratic convergence. A major result developed therein is that the

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Fréchet derivative at the desired invariant pair is nonsingular if and only if this invariant pair is simple. This conclusion is a generalization of the well-known fact that for linear eigenvalue problems, the Fréchet derivative at a single eigenpair is nonsingular if and only if this eigenvalue is simple. The nonsingularity of the Fréchet derivative is critical for the success of Newton's method. In Section 2, we briefly review some basic properties of invariant pairs.

In this paper, we study invariant pairs and present several new and important algebraic and analytical properties. We first show that the spectral structure, including the algebraic, partial, and geometric multiplicities together with all Jordan chains, of an eigenvalue of $T(\lambda)v = 0$ are completely resolved by the Jordan canonical form of a simple invariant pair that captures this eigenvalue. In other words, a nonlinear algebraic eigenvalue problem can be locally represented by a small linear matrix eigenvalue problem characterized by simple invariant pairs. These algebraic properties of invariant pairs are discussed in Section 3.

The second part of the paper concerns several analytical properties of invariant pairs, including approximation errors and perturbations of *simple* invariant pairs, and subspace projections (restrictions) of the nonlinear eigenproblem $T(\cdot)$ onto an approximate eigenspace. The first two issues are fundamental for the understanding of conditioning and sensitivity of simple invariant pairs. Given a simple invariant pair approximation with a small eigenresidual, we study conditions for the existence and uniqueness of a nearby exact invariant pair, and we give an error estimate of the approximate pair. The study of approximation errors is closely related to a perturbation analysis of exact invariant pairs. The result on subspace projections of a nonlinear eigenproblem shows that good eigenvalue approximations can be obtained provided that $T(\cdot)$ is projected onto accurate eigenspace approximations. In particular, the second order accuracy in eigenvalue approximation can be achieved by the two-sided block Rayleigh functional for non-defective eigenvalues. These analyses are presented in Section 4.

In Section 5, we study the matrix representation of the Fréchet derivative of the nonlinear eigenproblem formulated for invariant pairs, and we give an norm estimate of the inverse derivative. This estimate provides a quantitative description of the conditioning and sensitivity of the involved invariant pair. The structure of the Fréchet derivative is explored by studying the dimension of the kernel of a linear operator associated with $T(\cdot)$. We also briefly discuss upper bounds of the norm of the perturbed inverse Fréchet derivative involved in the analysis of approximation errors and perturbations of invariant pairs.

We give numerical examples in Section 6 to illustrate the approximation errors and perturbations of simple invariant pairs, and eigenvalue approximation accuracy achieved by block Rayleigh functionals. Finally, we summarize the paper in Section 7.

2. Preliminaries. Consider the general nonlinear algebraic eigenvalue problem

$$T(\lambda)v \equiv (f_1(\lambda)A_1 + f_2(\lambda)A_2 + \cdots + f_m(\lambda)A_m)\, v = 0, \tag{2.1}$$

where $f_1, \dots, f_m : \Omega \to \mathbb{C}$ are holomorphic functions defined on an open set $\Omega \subset \mathbb{C}$, and $A_1, \dots, A_m \in \mathbb{C}^{n\times n}$ are constant matrices. Here $\lambda \in \mathbb{C}$ is an eigenvalue, and $v \in \mathbb{C}^n \setminus \{0\}$ is the corresponding right eigenvector. To specify the scaling of v, a normalization condition $u^H v = 1$ with some fixed vector u is often imposed. The set of all eigenvalues of $T(\cdot)$ is called the spectrum of the nonlinear eigenproblem.

Let λ_0 be an eigenvalue of (2.1). The *geometric multiplicity* of λ_0, denoted by $geo_T(\lambda_0)$, is defined as $\dim(\ker(T(\lambda_0)))$; the *algebraic multiplicity* of λ_0, denoted by

$alg_T(\lambda_0)$, is the smallest integer i such that $\frac{\partial^i}{\partial\mu^i}\det(T(\mu))|_{\mu=\lambda_0} \neq 0$; see, for example, [12, Denition 7], [11, Definition A.3.4]. These definitions of multiplicities are identical to those for an eigenvalue of a square matrix.

Let (λ_0, v_0) be an eigenpair of the problem (2.1). An ordered collection of nonzero vectors $\{v_0, v_1, \ldots, v_{k-1}\}$ is called a *Jordan chain* of (2.1) or of the nonlinear eigenproblem $T(\cdot)$ corresponding to λ_0 if they satisfy

$$(2.2) \qquad \sum_{i=0}^{s} \frac{1}{i!} T^{(i)}(\lambda_0) v_{s-i} = 0 \quad \text{for } s = 1, \ldots, k-1, \quad \text{where } T^{(i)} = \frac{d^i}{d\mu^i} T(\mu).$$

Here, $v_1, \ldots, v_{k-1}$ are also called *generalized eigenvectors*; see [11, Definition A.3.5]. Suppose that (2.2) is satisfied for some $k = k_*$, and no more vectors can be introduced such that (2.2) is satisfied for $k = k_* + 1$, then k_* is the length of this Jordan chain, or a *partial multiplicity* of λ_0. If all Jordan chains corresponding to λ_0 are of length 1, then λ_0 is a *semi-simple* eigenvalue; otherwise it is *defective*. Semi-simple eigenvalues whose algebraic multiplicity is 1 are called *simple* eigenvalues.

In this paper, we only consider eigenvalues of finite algebraic multiplicity. In this case, [11, Corollary A.6.5] shows that in a neighborhood of λ_0,

$$(2.3) \qquad T(\mu) = N(\mu)\,\mathrm{diag}\left((\mu-\lambda_0)^{k_1}, (\mu-\lambda_0)^{k_2}, \ldots, (\mu-\lambda_0)^{k_g}, 1, \cdots, 1\right) M(\mu),$$

where $g = geo_T(\lambda_0)$, k_i are integers satisfying $1 \leq k_g \leq \cdots \leq k_1 < \infty$, $N(\mu)$ and $M(\mu)$ are holomorphic matrix functions in the neighborhood of λ_0, and $N(\lambda_0)$ are $M(\lambda_0)$ are nonsingular matrices. The diagonal matrix in (2.3) is called the (local) Smith form of $T(\mu)$. If the algebraic multiplicity of λ_0 is finite, it follows that λ_0 is the only point in the neighborhood of λ_0 at which $T(\cdot)$ is a singular matrix.

We note that the algebraic multiplicity of λ_0 can also be defined as the sum of all partial multiplicities of λ_0 (total length of all Jordan chains); see, e.g., [10] for matrices, and [11, Appendix A.] for nonlinear eigenproblems $T(\cdot)$. It can be shown that the two definitions are equivalent; see [11, Proposition A.6.4]. Both definitions are useful for the derivation of many fundamental theoretical results. For example, we can use the first definition of $alg_T(\lambda_0)$ to prove the following result:

PROPOSITION 2.1. *$geo_T(\lambda_0) \leq alg_T(\lambda_0)$.*

Proof. The conclusion holds trivially if $alg_T(\lambda_0) \geq n$. Assume that $alg_T(\lambda_0) < n$, and $geo_T(\lambda_0) = g$. Let $\{\varphi_1, \varphi_2, \cdots, \varphi_g\}$ be a basis of $\ker(T(\lambda_0))$, and choose linearly independent vectors $\{\xi_1, \xi_2, \ldots, \xi_{n-g}\}$ such that $B = [\varphi_1, \varphi_2, \ldots, \varphi_g, \xi_1, \xi_2, \ldots, \xi_{n-g}]$ is nonsingular. Because $T(\mu)$ is holomorphic in a neighborhood of λ_0, we have $T(\mu) = T(\lambda_0) + \sum_{k=1}^{\infty} T^{(k)}(\lambda_0)(\mu-\lambda_0)^k/k!$, and therefore

$$\begin{aligned} &\det(T(\mu)) = \det\left(T(\mu)B\right) \cdot \det\left(B^{-1}\right) \\ &= \det\left([T(\mu)\varphi_1, \ldots, T(\mu)\varphi_g, T(\mu)\xi_1, \ldots, T(\mu)\xi_{n-g}]\right) \cdot \det(B^{-1}) \\ &= \det\left([(\mu-\lambda_0)\psi_1, \ldots, (\mu-\lambda_0)\psi_g, T(\mu)\xi_1, \ldots, T(\mu)\xi_{n-g}]\right) \cdot \det(B^{-1}) \\ &= (\mu-\lambda_0)^g \det\left([\psi_1, \ldots, \psi_g, T(\mu)\xi_1, \ldots, T(\mu)\xi_{n-g}]\right) \cdot \det(B^{-1}), \end{aligned}$$

where $\psi_i = \sum_{k=1}^{\infty} \frac{T^{(k)}(\lambda_0)}{k!}(\mu-\lambda_0)^{k-1}\varphi_i$ $(1 \leq i \leq g)$ and $T(\mu)\xi_i$ $(1 \leq i \leq n-g)$ are holomorphic vector functions of μ in a neighborhood of λ_0, and $\psi_i \to T'(\lambda_0)\varphi_i$ as $\mu \to \lambda_0$. It follows that $\frac{d^j}{d\mu^j}\det(T(\mu))|_{\mu=\lambda_0} = 0$ if $j < g$, and thus $alg_T(\lambda_0) \geq g = geo_T(\lambda_0)$. ☐

To the best of our knowledge, the proof based on the first definition of $alg_T(\lambda_0)$ has not been given in the literature. Of course, the proposition holds trivially if

$alg_T(\lambda_0)$ is defined as the total length of Jordan chains corresponding to λ_0, because $geo_T(\lambda_0)$ is the number of Jordan chains.

The definition of an eigenpair (λ, v) can be naturally extended to allow treatment of several eigenpairs simultaneously. The extension, called invariant pairs, provide a convenient way for one to analyze multiple eigenpairs as an entity and develop numerical algorithms to compute them, especially for semi-simple and defective eigenvalues. The definition and preliminary properties of invariant pairs of the problem (2.1) were first discussed in [12]. In this paper, we study several important properties of invariant pairs, and we compare our results with those established since the 1970's for invariant subspaces of the standard eigenvalue problem $Av = \lambda v$. To prepare for the study, we briefly review the definitions and basic properties of invariant pairs.

A pair $(X, G) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$ is called *minimal* if there exists an integer $\ell \geq 1$ such that

$$U_\ell(X,G) \equiv \begin{bmatrix} X \\ XG \\ \vdots \\ XG^{\ell-1} \end{bmatrix} \tag{2.4}$$

has full column rank k. The smallest such ℓ is called the *minimality index* of (X, G). We can show that the minimality index of a minimal pair $(X, G) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$ is no greater than k.

A nonminimal pair can be replaced with a minimal pair. If $(X, G) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$ is nonminimal, then for a given ℓ, there exists a minimal pair $(\widehat{X}, \widehat{G}) \in \mathbb{C}^{n\times \hat{k}} \times \mathbb{C}^{\hat{k}\times \hat{k}}$, where $\hat{k} < k$, such that $\mathrm{span}\,(X) = \mathrm{span}(\widehat{X})$ and $\mathrm{span}\,(U_\ell(X, G)) = \mathrm{span}(U_\ell(\widehat{X}, \widehat{G}))$; see [2, Theorem 3]. This property allows us to restrict our discussion to minimal pairs.

Definition 2.2. *Consider $(V, L) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$, where the eigenvalues of L are contained in $\Omega \subset \mathbb{C}$. Then (V, L) is called an invariant pair of the nonlinear eigenvalue problem* (2.1) *if*

$$A_1 V f_1(L) + A_2 V f_2(L) + \cdots + A_m V f_m(L) = 0. \tag{2.5}$$

Note that in the case of matrix polynomials, i.e., $T(\cdot)$ is a polynomial of order ℓ, then the pair $(V, L) \in \mathbb{C}^{n\times \ell n} \times \mathbb{C}^{\ell n\times \ell n}$ satisfying (2.5) contains the complete spectral information for $T(\cdot)$, and it is called a standard pair of the matrix polynomial; see [6, Introduction]. In the general nonlinear case, we assume that the matrix functions $f_1(L), \ldots, f_m(L)$ are well-defined; see, e.g., [9] and [3, Definition 2.2]. For example, let $(\lambda_1, v_1), \ldots, (\lambda_k, v_k)$ be k eigenpairs of (2.1) where $\lambda_i \neq \lambda_j$ for $i \neq j$. It can be shown that (V, L) with $V = [v_1, \ldots, v_k]$ and $L = \mathrm{diag}(\lambda_1, \ldots, \lambda_k)$ is a minimal invariant eigenpair. Given a minimal invariant pair (V, L), one can show that for any nonsingular $Z \in \mathbb{C}^{k\times k}$, $(VZ, Z^{-1}LZ)$ is also a minimal invariant pair, and the eigenvalues of L are those of the problem (2.1); that is, $\Lambda(L) \subset \Lambda(T(\cdot))$, where Λ stands for the spectrum of a matrix or nonlinear eigenproblem. Note that for the standard eigenvalue problem where $T(\mu) = \mu I - A$, it is easy to see that an eigenpair (V, L) with $AV = VL$ is minimal, and $\Lambda(L) \subset \Lambda(A)$. Since $\Lambda(L) \subset \Lambda(T(\cdot))$, we can have the following definition.

Definition 2.3. *An invariant pair (V, L) for problem* (2.1) *is called simple if (V, L) is minimal and the algebraic multiplicity of each eigenvalue of L is identical to the algebraic multiplicity of this eigenvalue of the problem* (2.1).

To specify the scaling of V for a given invariant pair (V, L), we choose an integer ℓ no less than the minimality index of (V, L) such that $U_\ell(V, L)$ defined in (2.4) has full column rank k. Define

$$(2.6) \qquad W = \begin{bmatrix} W_0 \\ W_1 \\ \vdots \\ W_{\ell-1} \end{bmatrix} = U_\ell(V, L) \left(U_\ell(V, L)^H U_\ell(V, L)\right)^{-1} \in \mathbb{C}^{\ell n \times k},$$

such that $W^H U_\ell(V, L) = I_k$. Let $\mathbb{C}_\Omega^{k\times k}$ be the set of $k \times k$ complex matrices whose spectrum lies in Ω. Kressner [12] observed that the invariant pair (V, L) is a root of the following matrix operators $\mathbb{T} : \mathbb{C}^{n\times k} \times \mathbb{C}_\Omega^{k\times k} \to \mathbb{C}^{n\times k}$ and $\mathbb{V} : \mathbb{C}^{n\times k} \times \mathbb{C}_\Omega^{k\times k} \to \mathbb{C}^{k\times k}$:

$$(2.7) \qquad \begin{cases} \mathbb{T} : (X, G) \to A_1 X f_1(G) + A_2 X f_2(G) + \cdots + A_m X f_m(G) \\ \mathbb{V} : (X, G) \to W^H U_\ell(X, G) - I_k \end{cases} .$$

The Fréchet derivative of $\mathbb{T}$ and $\mathbb{V}$ at (X, G) are the operators defined as follows:

$$(2.8) \begin{cases} \mathbb{DT}_{(X,G)} : (\Delta X, \Delta G) \to \mathbb{T}(\Delta X, G) + \sum_{j=1}^{m} A_j X \mathbb{D}f_{j(G)}(\Delta G) \\ \mathbb{DV}_{(X,G)} : (\Delta X, \Delta G) \to W_0^H \Delta X + \sum_{j=1}^{\ell-1} W_j^H \left(\Delta X G^j + X[\mathbb{D}G^j](\Delta G)\right) \end{cases} .$$

Here, $\mathbb{D}f_{j(G)}$ is the Fréchet derivative of the matrix function $G \to f_j(G)$, and $\mathbb{D}G^j$ is the Fréchet derivative of the matrix function $G \to G^j$.

The following major result given in [12] shows that a simple invariant pair (V, L) is a simple root of the nonlinear matrix equation $(\mathbb{T}(X, G), \mathbb{V}(X, G)) = (0, 0)$.

Theorem 2.4. [12, Theorem 10] *Let (V, L) be a minimal invariant pair of the problem* (2.1)*. Then (V, L) is simple if and only if the associated Fréchet derivative*

$$(2.9) \qquad \mathbb{L}_{(V,L)} : (\Delta X, \Delta G) \to \left(\mathbb{DT}_{(V,L)}(\Delta X, \Delta G), \mathbb{DV}_{(V,L)}(\Delta X, \Delta G)\right)$$

is invertible, where $\mathbb{DT}$ and $\mathbb{DV}$ are defined in (2.8)*.*

Simple invariant pairs of the nonlinear eigenproblem $T(\cdot)$ are natural generalizations of simple invariant subspaces and corresponding projections of square matrices. The major characteristic of both entities is that their corresponding spectra are disjoint with the rest of the spectrum of the original eigenvalue problem. As a result, they change analytically under analytic perturbation of the eigenvalue problem. This property guarantees that the numerical computation of simple invariant pairs is a well-posed problem. In particular, iterative algorithms for computing simple invariant subspaces and simple invariant pairs provide reliable approximations to degenerate (semi-simple or defective) eigenvalues and associated eigenspaces. In the following sections, we investigate several important properties of invariant pairs.

3. Some algebraic properties of simple invariant pairs. This section concerns a few fundamental algebraic properties of simple invariant pairs (V, L) of (2.1). We show that the spectral structure (algebraic, partial, and geometric multiplicities, and Jordan chains) of an eigenvalue λ_0 of the eigenvalue problem $T(\lambda)v = 0$ is completely resolved by a simple invariant pair that captures this eigenvalue.

Theorem 3.1. *Suppose that (V, L) is a simple invariant pair of* (2.1)*, $\lambda_0 \in \Lambda(L)$, and $J_L = Z^{-1}LZ$ is the Jordan canonical form of L. Assume that J_L has g Jordan blocks corresponding to λ_0, each of size $k_i \times k_i$ $(1 \le i \le g)$. Then there are exactly g Jordan chains of $T(\cdot)$ corresponding to λ_0, the length of each is k_i, and $geo_T(\lambda_0) = g$.*

Proof. Without loss of generality, let

$$J_L = \begin{bmatrix} J_{k_1}(\lambda_0) & & & & \\ & J_{k_2}(\lambda_0) & & & \\ & & \ddots & & \\ & & & J_{k_g}(\lambda_0) & \\ & & & & J(\lambda_{other}) \end{bmatrix}, \; J_{k_i}(\lambda_0) = \begin{bmatrix} \lambda_0 & 1 & & & \\ & \lambda_0 & 1 & & \\ & & \ddots & \ddots & \\ & & & \lambda_0 & 1 \\ & & & & \lambda_0 \end{bmatrix}_{k_i \times k_i},$$

where $J(\lambda_{other})$ is the block diagonal matrix of Jordan blocks corresponding to other eigenvalues of L. Let $alg_L(\lambda_0)$ be the algebraic multiplicity of λ_0 as an eigenvalue of L. Then, by the definition of simple invariant pairs and the structure of J_L, we have $alg_T(\lambda_0) = alg_L(\lambda_0) = k_1 + k_2 + \cdots + k_g$.

Since (V, L) is an invariant pair, we know from Section 2 that $(VZ, Z^{-1}LZ) = (VZ, J_L)$ is an invariant pair, and $U_\ell(VZ, J_L) = U_\ell(V, L)Z$ has full column rank k with minimality index ℓ. For the sake of brevity of notation, let

$$VZ = \left[\varphi_{1,0}, \varphi_{1,1}, \ldots, \varphi_{1,k_1-1}, \varphi_{2,0}, \ldots, \varphi_{2,k_2-1}, \ldots, \varphi_{g,0}, \ldots, \varphi_{g,k_g-1}, \Phi_{other}\right];$$

that is, we partition VZ according to the order and size of the Jordan blocks $\{J_{k_i}(\lambda_0)\}$. Consider the collection of vectors $\varphi_{1,0}, \varphi_{2,0}, \ldots, \varphi_{g,0}$. These vectors must be linearly independent; otherwise the 1st, (k_1+1)st, ..., and $(k_1+\cdots+k_{g-1}+1)$st column vectors of $U_\ell(VZ, J_L)$ (corresponding to the first columns of $J_{k_1}(\lambda_0), J_{k_2}(\lambda_0), \ldots, J_{k_g}(\lambda_0)$), namely,

$$\begin{bmatrix} \varphi_{1,0} \\ \lambda_0\varphi_{1,0} \\ \vdots \\ \lambda_0^{\ell-1}\varphi_{1,0} \end{bmatrix}, \begin{bmatrix} \varphi_{2,0} \\ \lambda_0\varphi_{2,0} \\ \vdots \\ \lambda_0^{\ell-1}\varphi_{2,0} \end{bmatrix}, \ldots, \begin{bmatrix} \varphi_{g,0} \\ \lambda_0\varphi_{g,0} \\ \vdots \\ \lambda_0^{\ell-1}\varphi_{g,0} \end{bmatrix},$$

are linearly dependent, contradicting the fact that $U_\ell(VZ, J_L)$ has full column rank.

Now note that the matrix function $f(J_L)$ is defined as (see, e.g., [3],[9])

$$f(J_L) = \begin{bmatrix} f(J_{k_1}(\lambda_0)) & & & & \\ & f(J_{k_2}(\lambda_0)) & & & \\ & & \ddots & & \\ & & & f(J_{k_g}(\lambda_0)) & \\ & & & & f(J(\lambda_{other})) \end{bmatrix}, \tag{3.1}$$

where

$$f(J_{k_i}(\lambda_0)) = \begin{bmatrix} f(\lambda_0) & f'(\lambda_0) & \frac{f''(\lambda_0)}{2!} & \cdots & \frac{f^{(k_i-1)}(\lambda_0)}{(k_i-1)!} \\ & f(\lambda_0) & f'(\lambda_0) & & \frac{f^{(k_i-2)}(\lambda_0)}{(k_i-2)!} \\ & & \ddots & \ddots & \vdots \\ & & & f(\lambda_0) & f'(\lambda_0) \\ & & & & f(\lambda_0) \end{bmatrix} \quad (1 \le i \le g). \tag{3.2}$$

Since (VZ, J_L) is an invariant pair of the problem (2.1), we can substitute (V, L) with (VZ, J_L) in (2.5). Considering the 1st, (k_1+1)st, ..., and $(k_1+\cdots+k_{g-1}+1)$st columns, we have from (3.1) and (3.2) that

$$\sum_{j=1}^{m} A_j \varphi_{i,0} f_j(\lambda_0) = T(\lambda_0)\varphi_{i,0} = 0 \quad \text{for } 1 \le i \le g.$$

Similarly, we see from other columns that

$$(3.3)\qquad \sum_{j=1}^{m} A_j \sum_{r=0}^{s_i} \varphi_{i,s_i-r} \frac{f_j^{(r)}(\lambda_0)}{r!} = \sum_{r=0}^{s_i} \frac{1}{r!} T^{(r)}(\lambda_0)\varphi_{i,s_i-r} = 0,$$

for $i = 1, 2, \ldots, g$, and $s_i = 1, 2, \ldots, k_i - 1$. That is, $\varphi_{1,0}, \varphi_{2,0}, \ldots, \varphi_{g,0} \in \ker(T(\lambda_0))$, and therefore $geo_T(\lambda_0) \geq g$. Also, $\{\varphi_{1,0}, \ldots, \varphi_{1,k_1-1}\}$, $\{\varphi_{2,0}, \ldots, \varphi_{2,k_2-1}\}$, $\ldots$, and $\{\varphi_{g,0}, \ldots, \varphi_{g,k_g-1}\}$ form g Jordan chains corresponding to λ_0.

Note that the algebraic multiplicity of λ_0 as an eigenvalue of L is $alg_L(\lambda_0) = \sum_{i=1}^{g} k_i$. From (3.3) and the definition (2.2), $k_1, k_2, \ldots, k_g$ are lower bounds of the lengths of the g Jordan chains, because there may exist additional generalized eigenvectors such that the length of one of these Jordan chains is greater than k_i. Since $alg_T(\lambda_0)$ equals the total length of all (possibly more than g) Jordan chains corresponding to λ_0, we have $alg_L(\lambda_0) \leq alg_T(\lambda_0)$. For a simple invariant pair (V, L), since $alg_L(\lambda_0) = alg_T(\lambda_0)$, we see that there do not exist any additional Jordan chains corresponding to λ_0, and there do not exist additional generalized eigenvectors such that the length of any of these g Jordan chains is greater than k_i. Therefore $geo_T(\lambda_0) = g$, and the length of each Jordan chain is k_i $(1 \leq i \leq g)$. This completes the proof. □

Theorem 3.1 shows that through simple invariant pairs, the nonlinear algebraic eigenvalue problem can be *locally* represented by a small matrix eigenvalue problem. This insight is obtained by exploring the Jordan canonical form of the matrix L, its connection to matrix functions and the definition of Jordan chains.

4. Some analytical properties of invariant pairs. In this section, we study several analytical properties of invariant pairs. First, given an approximate invariant pair (X, G), we discuss the conditions for the existence and uniqueness of a nearby exact invariant pair (V, L), and we explore the error of (X, G) as an approximation of (V, L). The study of approximation error leads to a perturbation analysis of an exact invariant pair (V, L). In addition, we consider the projection (restriction) of $T(\cdot)$ onto an approximate eigenspace. This projection is a block generalization of the nonlinear Rayleigh functional [23], and it provides eigenvalue approximations associated with the approximate eigenspace.

The major mathematical tool we will use to study the analytical properties of invariant pairs is the Newton-Kantorovich theorem; see, e.g., [8], [19]. For a nonlinear functional F defined on Banach spaces whose Fréchet derivative is Lipschitz continuous, the theorem states that, given a vector u_0 for which $F'(u_0)$ is nonsingular and its inverse is bounded and, moreover, $\|F(u_0)\|$ is sufficiently small, there exists a unique root of F nearby.

THEOREM 4.1 (Newton-Kantorovich). *Let Y and Z be two Banach spaces, and D an open convex subset of Y. Let $F : D \to Z$ be Fréchet differentiable on D. Suppose that there exists $\gamma > 0$ such that $\|F'(u_a) - F'(u_b)\| \leq \gamma \|u_a - u_b\|$ for all $u_a, u_b \in D$. Assume that $u_0 \in D$ is such that $[F'(u_0)]^{-1} : Z \to Y$ exists, and there exist $\kappa > 0$, $\delta > 0$ such that $\left\|[F'(u_0)]^{-1}\right\| \leq \kappa$, and $\left\|[F'(u_0)]^{-1} F(u_0)\right\| \leq \delta$. Suppose that $B(u_0, d_s) = \{u : \|u - u_0\| \leq d_s\} \subset D$, where $d_s = 2(1 - \sqrt{1-h})\delta/h$, and let $h \equiv 2\gamma\kappa\delta$. If $h \leq 1$, then*

1. *the Newton iterates $u_{n+1} = u_n - [F'(u_n)]^{-1} F(u_n)$ exist and $u_n \in B(u_0, d_s)$ for all n;*
2. *$u^* = \lim x_n$ exists, $F(u^*) = 0$, and $u^* \in \overline{B(u_0, d_s)} \subset \overline{D}$;*
3. *u^* is the only solution of $F(u) = 0$ in $B(u_0, d_l) \cap D$ if $h < 1$, and in $\overline{B(u_0, d_l)}$ if $h = 1$, where $d_l = 2(1 + \sqrt{1-h})\delta/h$.*

Remark 4.2. In Theorem 4.1, it is worth noting that we can let $\kappa \equiv \left\| [F'(u_0)]^{-1} \right\|$ and $\delta \equiv \left\| [F'(u_0)]^{-1} F(u_0) \right\|$ to obtain the optimal bounds. In fact, by such definitions of κ and δ, $h \equiv 2\kappa\gamma\delta$ attains its minimum value, so that there is a greater possibility to satisfy $h \leq 1$; also, $d_s = \frac{2\delta}{1+\sqrt{1-2\kappa\gamma\delta}}$ is minimized for the bound of $\|u_0 - u^*\|$, and $d_l = \frac{1+\sqrt{1-2\kappa\gamma\delta}}{\kappa\gamma}$ is maximized for radius of the ball in which u^* is the unique root of F. In the following analysis, we will use such definitions for κ and δ.

To prepare for the analysis of approximation errors and perturbations of invariant pairs, consider the Banach space $\mathcal{B}$ of matrix pairs $(X, G) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$. Define

$$\begin{aligned} \|(X,G)\| &\equiv \left\| \begin{bmatrix} X \\ G \end{bmatrix} \right\|_F = \left\| \begin{bmatrix} vec(X) \\ vec(G) \end{bmatrix} \right\|_2, \\ \|X\| &\equiv \|X\|_F = \|vec(X)\|_2, \quad \text{and} \quad \|G\| \equiv \|G\|_F = \|vec(G)\|_2, \end{aligned} \tag{4.1}$$

where $vec(\cdot)$ is the standard vectorization of a matrix. It follows that $\|X\| \leq \|(X,G)\|$ and $\|G\| \leq \|(X,G)\|$.

Suppose that a function $F : \mathcal{B} \to \mathcal{B}$ is Fréchet differentiable. Its Fréchet derivative $\mathbb{DF} : \mathcal{B} \to \mathcal{B}$ is a linear transformation whose norm is defined in the usual manner

$$\|\mathbb{DF}\| \equiv \max_{\|(\Delta X, \Delta G)\| \neq 0} \frac{\|\mathbb{DF}(\Delta X, \Delta G)\|}{\|(\Delta X, \Delta G)\|}. \tag{4.2}$$

Since $\mathcal{B}$ is a Banach space of dimension $nk + k^2 = (n+k)k$, the linear transformation $\mathbb{DF}$ defined on $\mathcal{B}$ can be represented by an $(n+k)k \times (n+k)k$ matrix. Given the definition of the "vector" norm $\|(X,G)\|$ in (4.1), we can see that $\|\mathbb{DF}\|$ defined in (4.2) equals the 2-norm of the matrix representation of $\mathbb{DF}$. In fact, any consistent matrix norm can be used to define $\|(X,G)\|$, $\|X\|$ and $\|G\|$.

The treatment of the "eigenvector part" and "eigenvalue part" as an entity seems most natural in the our setting. However, one needs to realize that this treatment has certain shortcomings. For example, $\|(X-V, G-L)\|$ may not capture wide-varying magnitudes in the eigenvector and the eigenvalue parts; for example, if $\|X - V\| \gg \|G-L\|$, an accurate estimate of $\|(X-V, G-L)\|$ is a serious overestimate of $\|G-L\|$. In addition, for two equivalent invariant pairs (V_1, L_1) and (V_2, L_2) such that $V_2 = V_1 S$ and $L_2 = S^{-1} L_1 S$ for a nonsingular S, $\|(V_1 - V_2, L_1 - L_2)\|$ does not reveal the equivalence of the two pairs. Another issue is the loss of scale-invariance. An invariant pair (V, L) of $T(\lambda)v = 0$ corresponds to $(V, \frac{1}{\alpha} L)$ of the scaled problem $T(\alpha\lambda)v = 0$, and thus the bounds on approximation errors and perturbations of invariant pairs of the original problem can not be converted to the bounds for the scaled problem by simple scaling. Nevertheless, to the best of our knowledge, our results based on invariant pairs and their norms provide new insights into the properties of multiple eigenpairs as an entity that are not well-understood by alternative approaches.

4.1. Error estimate of approximate invariant pairs. In this section, we consider an approximate invariant pair (X, G) of the problem (2.1) for which the eigenresidual norm $\|\mathbb{T}(X,G)\|$ is small. We give conditions for the existence and uniqueness of a nearby exact invariant pair (V, L) and the approximation error of (X, G). We will see later that our result is very similar to that of eigenpairs of *matrices* developed by Stewart [24], [25], which is restated in the following proposition.

Proposition 4.3. [27, Chapter 4, Theorem 2.12] *Let X be a set of orthonormal vectors that span an approximate invariant subspace of $A \in \mathbb{C}^{n\times n}$, and $[X \;\; X_\perp]$ be a* *unitary matrix. Let $G = X^H AX$ and $M = X_\perp^H AX_\perp$ be the Rayleigh quotients associated with X and $X_\perp$, respectively. Define $S^H = X^H A - GX^H$ and the eigenresidual $R = AX - XG$. Suppose that $4\|R\|\|S\| \le sep^2(G, M)$ in the 2-norm, where*

$$sep(G, M) = \inf_{\|Q\|\neq 0} \frac{\|\mathbb{S}(Q)\|}{\|Q\|} = \left(\sup_{\|Q\|\neq 0} \frac{\|\mathbb{S}^{-1}(Q)\|}{\|Q\|} \right)^{-1} = \|\mathbb{S}^{-1}\|^{-1}, \tag{4.3}$$

and

$$\mathbb{S} : Q \to QG - MQ \tag{4.4}$$

is a linear Sylvester operator. Then there exists a simple eigenpair (V, L) of A, i.e., $AV = VL$ and $\Lambda(L) \cap (\Lambda(A) \setminus \Lambda(L)) = \emptyset$, such that

$$\|G - L\| \le \frac{2\|R\|\|S\|}{sep(G, M)}, \quad \textit{and} \quad \tan \angle(X, V) \le \frac{2\|R\|}{sep(G, M)}, \tag{4.5}$$

where $\angle(X, V)$ stands for the largest canonical angle between span$\{X\}$ *and* span$\{V\}$*; see, e.g.,* [7, Chapter 2.6], [26, Chapter 1.4.5].

To prepare for the study of approximation errors of invariant pairs, we first review the Mean Value Theorem in a Banach space (see, e.g., [20, Section 3.2]), and we discuss a sufficient condition for the Lipschitz continuity of the Fréchet derivative $\mathbb{L}$.

Lemma 4.4 (Mean Value Theorem). *Let Y and Z be two Banach spaces, and D an open convex subset of Y containing u_a and u_b. Define*

$$\begin{aligned}(u_a, u_b) &= \{u : u = \alpha u_a + (1 - \alpha)u_b,\ 0 < \alpha < 1\}, \textit{ and} \\ [u_a, u_b] &= \{u : u = \alpha u_a + (1 - \alpha)u_b,\ 0 \le \alpha \le 1\}.\end{aligned}$$

Let $F : D \to Z$ be a continuous functional on $[u_a, u_b]$ whose Fréchet derivative $\mathbb{DF}$ exists for all $u \in (u_a, u_b)$. Then

$$\|F(u_b) - F(u_a)\| \le \sup_{u\in(u_a,u_b)} \|\mathbb{DF}(u)\|\|u_b - u_a\|.$$

The Lipschitz continuity of the Fréchet derivative $\mathbb{L}$ (see (2.8)) can be established by the following lemma.

Lemma 4.5. *Suppose that the Fréchet derivatives of the functions $\{f_j\}$ in* (2.1) *are Lipschitz continuous, i.e., there exists $\gamma_j > 0$ such that $\left\|\mathbb{D}f_{j(G_1)} - \mathbb{D}f_{j(G_2)}\right\| \le \gamma_j\|G_1 - G_2\|$ for all $G_1, G_2 \in \mathbb{C}_\Omega^{k\times k}$. Let $\mathbb{C}_\Gamma^{n\times k} \subset \mathbb{C}^{n\times k}$ be a convex and bounded set. If Ω is bounded and $\mathbb{C}_\Omega^{k\times k}$ is convex, then the Fréchet derivative $\mathbb{L}_{(X,G)} = \left(\mathbb{DT}_{(X,G)}, \mathbb{DV}_{(X,G)}\right)$ is Lipschitz continuous in $\mathbb{C}_\Gamma^{n\times k} \times \mathbb{C}_\Omega^{k\times k}$.*

Proof. Note that $\mathbb{L}_{(X,G)}$ is Lipschitz continuous if $\mathbb{DT}$ and $\mathbb{DV}$ defined in (2.8) are Lipschitz continuous. We first show the Lipschitz continuity of $\mathbb{DT}$. From (2.8), for any $(X_1,G_1),(X_2,G_2)\in\mathbb{C}_\Gamma^{n\times k}\times\mathbb{C}_\Omega^{k\times k}$, we have

$$\begin{aligned}
&\left\|\mathbb{DT}_{(X_1,G_1)}(\Delta X,\Delta G)-\mathbb{DT}_{(X_2,G_2)}(\Delta X,\Delta G)\right\|\\
&=\left\|\mathbb{T}(\Delta X,G_1)-\mathbb{T}(\Delta X,G_2)+\sum_{j=1}^m A_j\left(X_1\mathbb{D}f_{j(G_1)}(\Delta G)-X_2\mathbb{D}f_{j(G_2)}(\Delta G)\right)\right\|\\
&\le\left\|\sum_{j=1}^m A_j\Delta X\left(f_j(G_1)-f_j(G_2)\right)\right\|\\
&\qquad+\left\|\sum_{j=1}^m A_j\left((X_1-X_2)\mathbb{D}f_{j(G_2)}(\Delta G)+X_1\left(\mathbb{D}f_{j(G_1)}(\Delta G)-\mathbb{D}f_{j(G_2)}(\Delta G)\right)\right)\right\|\\
&\le\sum_{j=1}^m\|A_j\|\sup_{G\in(G_1,G_2)}\left\|\mathbb{D}f_{j(G)}\right\|\|G_1-G_2\|\|\Delta X\|\qquad\text{(using Lemma 4.4)}\\
&\qquad+\sum_{j=1}^m\|A_j\|\left(\|X_1-X_2\|\left\|\mathbb{D}f_{j(G_2)}\right\|\|\Delta G\|+\|X_1\|\gamma_j\|G_1-G_2\|\|\Delta G\|\right)\\
&\le\sum_{j=1}^m\|A_j\|\sup_{G\in(G_1,G_2)}\left\|\mathbb{D}f_{j(G)}\right\|\|(X_1-X_2,G_1-G_2)\|\|(\Delta X,\Delta G)\|\\
&\qquad+\sum_{j=1}^m\|A_j\|\left(\left\|\mathbb{D}f_{j(G_2)}\right\|+\gamma_j\|X_1\|\right)\|(X_1-X_2,G_1-G_2)\|\|(\Delta X,\Delta G)\|.
\end{aligned}$$

It then follows that

$$\begin{aligned}
&\left\|\mathbb{DT}_{(X_1,G_1)}-\mathbb{DT}_{(X_2,G_2)}\right\|\\
&=\sup_{(\Delta X,\Delta G)\neq 0}\frac{\left\|\mathbb{DT}_{(X_1,G_1)}(\Delta X,\Delta G)-\mathbb{DT}_{(X_2,G_2)}(\Delta X,\Delta G)\right\|}{\|(\Delta X,\Delta G)\|}\\
&\le\sum_{j=1}^m\|A_j\|\left(\sup_{G\in(G_1,G_2)}\left\|\mathbb{D}f_{j(G)}\right\|+\|\mathbb{D}f_{j(G_2)}\|+\gamma_j\|X_1\|\right)\|(X_1-X_2,G_1-G_2)\|\\
&\equiv\gamma_{DT}\|(X_1-X_2,G_1-G_2)\|.
\end{aligned}$$

Here, $\gamma_{DT}=\sum_{j=1}^m\|A_j\|\left(\sup_{G\in(G_1,G_2)}\|\mathbb{D}f_{j(G)}\|+\|\mathbb{D}f_{j(G_2)}\|+\gamma_j\|X_1\|\right)$ is bounded, because both $\|\mathbb{D}f_j\|$ and $\|X_1\|$ are bounded ($\mathbb{D}f_j$ is Lipschitz continuous on the bounded set $\mathbb{C}_\Omega^{k\times k}$, and X_1 belongs to the bounded set $\mathbb{C}_\Gamma^{n\times k}$).

The proof of the Lipschitz continuity of $\mathbb{DV}$ follows the lines of that for $\mathbb{DT}$, and is therefore omitted. The lemma is thus established. □

Let (X,G) be an approximate invariant pair such that $W^HU_\ell(X,G)$ is nonsingular. Define $\widetilde{X}=X(W^HU_\ell(X,G))^{-1}$ and $\widetilde{G}=(W^HU_\ell(X,G))G(W^HU_\ell(X,G))^{-1}$. We see that $\mathbb{T}(\widetilde{X},\widetilde{G})=\mathbb{T}(X,G)(W^HU_\ell(X,G))^{-1}$, and $W^HU_\ell(\widetilde{X},\widetilde{G})-I_k=0$. Because $\widetilde{X}$ and X span the same subspace, and $\widetilde{G}$ and G have identical spectrum, $(\widetilde{X},\widetilde{G})$ and (X,G) are "equivalent" approximate invariant pairs. Therefore, from now on, it suffices to consider approximate invariant pairs (X,G) satisfying $W^HU_\ell(X,G)-I_k=0$.

We are now ready to present a theorem giving an error estimate of an approximate invariant pair (X,G) of the nonlinear eigenvalue problem (2.1).

Theorem 4.6. *Let $(X,G)\in\mathbb{C}_\Gamma^{n\times k}\times\mathbb{C}_\Omega^{k\times k}$ satisfying $W^HU_\ell(X,G)-I_k=0$ be an approximate minimal invariant pair of* (2.1)*, where $\mathbb{C}_\Gamma^{n\times k}$ is bounded and convex,* *and $\mathbb{C}_{\Omega}^{k\times k}$ is open and convex with bounded Ω. Suppose that the Fréchet derivative $\mathbb{L}_{(X,G)}$ is nonsingular, and $\kappa = \left\|\mathbb{L}_{(X,G)}^{-1}\right\|$ is finite, and there exists $\gamma > 0$ such that $\left\|\mathbb{L}_{(X_1,G_1)} - \mathbb{L}_{(X_2,G_2)}\right\| \leq \gamma\|(X_1-X_2, G_1-G_2)\|$ for all $(X_1, G_1), (X_2, G_2) \in \mathbb{C}_{\Gamma}^{n\times k} \times \mathbb{C}_{\Omega}^{k\times k}$. Suppose that $\mathbb{T}(X,G)$ is small in norm such that $\delta = \left\|\mathbb{L}_{(X,G)}^{-1}(\mathbb{T}(X,G), 0)\right\|$ satisfies $h \equiv 2\kappa\gamma\delta \leq 1$, and that $B((X,G), \frac{2\delta}{1+\sqrt{1-h}}) \subset \mathbb{C}_{\Gamma}^{n\times k} \times \mathbb{C}_{\Omega}^{k\times k}$, then there is a unique invariant pair (V, L) of (2.1) in $B((X,G), \frac{1+\sqrt{1-h}}{\kappa\gamma}) \cap \mathbb{C}_{\Gamma}^{n\times k} \times \mathbb{C}_{\Omega}^{k\times k}$ (if $h < 1$) or in $\overline{B((X,G), \frac{1}{\kappa\gamma})}$ (if $h = 1$) with $\|(X-V, G-L)\| \leq \frac{2\delta}{1+\sqrt{1-h}}$.*

Proof. Consider the Banach spaces $D = \mathbb{C}_{\Gamma}^{n\times k} \times \mathbb{C}_{\Omega}^{k\times k}$, $Z = \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$, and the functionals $F : (X,G) \to (\mathbb{T}(X,G), \mathbb{V}(X,G))$, $F' : (\Delta X, \Delta G) \to \mathbb{L}_{(X,G)}(\Delta X, \Delta G)$. Let $u_0 = (X,G)$. The theorem can be established by applying Theorem 4.1. $\square$

Theorem 4.6 gives an explicit bound of the approximation error of (X,G), namely, $\|(X-V, G-L)\| \leq d_s \equiv \frac{2\delta}{1+\sqrt{1-h}}$. Since $0 \leq h \leq 1$, we can see that

$$\delta \leq d_s \leq 2\delta = 2\left\|\mathbb{L}_{(X,G)}^{-1}(\mathbb{T}(X,G), 0)\right\| \leq 2\left\|\mathbb{L}_{(X,G)}^{-1}\right\|\|\mathbb{T}(X,G)\|, \tag{4.6}$$

which is very similar to the error estimate of approximate invariant subspaces (4.5). Both error estimates are proportional to the eigenresidual norm of the approximate invariant pair, and inversely proportional to the reciprocal of the norm of an inverse linear operator; see (2.8) and (2.9), (4.3) and (4.4), respectively, for the two linear operators involved. In both cases, by an analogy to the singular values of a nonsingular matrix, we see that the reciprocal of the norm of the inverse operator is essentially the smallest singular value of the original operator. This quantity measures the separation between the spectrum approximation G and the rest of the spectrum of the eigenvalue problem. The smaller this separation is, the larger the approximation error could be. In Section 5, we give an estimate of this separation for the case where a semi-simple eigenvalue is the only distinct eigenvalue present in an invariant pair.

Note that if $\|X\|$ is considerably smaller or larger than $\|V\|$, then the upper bound of $\|(X-V, G-L)\|$ given in Theorem 4.6 can be a significant overestimate of $\angle(X,V)$. This overestimate can be avoided for linear eigenvalue problems by considering an unitary block triangularization of a matrix or a matrix pair and orthogonal projection of the exact invariant subspace onto the approximate invariant subspace; see, e.g., [24], [25]. Similarly, for nonlinear eigenvalue problems, one may consider the use of an orthogonal projection of $X-V$ onto V, but this approach does not yield an explicit sharper error estimate; see, e.g., [2]. If X and V are appropriately normalized such that $\|X\| \approx \|V\|$, it is natural to expect d_s as a reasonable upper bound of $\angle(X,V)$, provided that $\|X-V\|$ is not much smaller than $\|G-L\|$.

4.2. Perturbation analysis of simple invariant pairs. In this section, we develop a perturbation analysis of simple invariant pairs of the nonlinear eigenvalue problem (2.1) with focus on their condition number, and we compare our result with the perturbation analysis of simple eigenpairs of a matrix given by Stewart [25]. We first introduce a block diagonalization of a matrix and review Stewart's analysis.

LEMMA 4.7. *Suppose that (V_1, L) is an invariant pair of $A \in \mathbb{C}^{n\times n}$, that is, $AV_1 - V_1L = 0$ where V_1 has orthonormal columns and $L = V_1^H AV_1 \in \mathbb{C}^{k\times k}$. Choose $W_2 \in \mathbb{C}^{n\times(n-k)}$ such that $[V_1\ W_2]$ is unitary, and let $M = W_2^H AW_2$. If (V_1, L) is simple, i.e., $\Lambda(L) \cap \Lambda(M) = \emptyset$, then there exists matrices $V_2 \in \mathbb{C}^{n\times(n-k)}$ and*

$W_1 \in \mathbb{C}^{n\times k}$ *such that* $[W_1\, W_2]^H = [V_1\, V_2]^{-1}$, *and* A *can be block diagonalized as*

$$A = [V_1 \;\; V_2] \begin{bmatrix} L & \\ & M \end{bmatrix} \begin{bmatrix} W_1^H \\ W_2^H \end{bmatrix}. \tag{4.7}$$

Proof. Suppose that A has a Jordan canonical form

$$A = PJP^{-1} = [P_1 \;\; P_2] \begin{bmatrix} J_1 & \\ & J_2 \end{bmatrix} \begin{bmatrix} Q_1^H \\ Q_2^H \end{bmatrix}.$$

It is then easy to see that A can be decomposed as (4.7), where

$$\begin{aligned} &V_1 = P_1(P_1^H P_1)^{-1/2}, \;\; V_2 = P_2(Q_2^H Q_2)^{1/2}, \\ &L = (P_1^H P_1)^{1/2} J_1 (P_1^H P_1)^{-1/2}, \;\; M = (Q_2^H Q_2)^{-1/2} J_2 (Q_2^H Q_2)^{1/2}, \\ &W_1 = Q_1(P_1^H P_1)^{1/2}, \;\; W_2 = Q_2(Q_2^H Q_2)^{-1/2}, \end{aligned}$$

and both V_1 and W_2 have orthonormal columns. ∎

PROPOSITION 4.8. [27, Chapter 4, Theorem 2.13] *Let* $A \in \mathbb{C}^{n\times n}$ *have the decomposition as* (4.7), *where* $\Lambda(L) \cap \Lambda(M) = \emptyset$. *Letting* $\widetilde{A} = A + E$, *we have*

$$\begin{bmatrix} W_1^H \\ W_2^H \end{bmatrix} (A+E)\, [V_1 \;\; V_2] = \begin{bmatrix} L + F_{11} & F_{12} \\ F_{21} & M + F_{22} \end{bmatrix},$$

where $F_{11} = W_1^H E V_1$, $F_{12} = W_1^H E V_2$, $F_{21} = W_2^H E V_1$ *and* $F_{22} = W_2^H E V_2$. *Suppose that* $4\|F_{12}\|\|F_{21}\| \le sep^2(L + F_{11}, M + F_{22})$, *then there is* $S \in \mathbb{C}^{(n-k)\times k}$ *satisfying* $\|S\| \le \frac{2\|F_{21}\|}{sep(L+F_{11}, M+F_{22})}$ *such that*

$$(\widetilde{L}, \widetilde{V}_1) = (L + F_{11} + F_{12}S,\, V_1 + V_2 S)$$

is a simple right eigenpair of $\widetilde{A}$, *i.e.,* $\widetilde{A}\widetilde{V}_1 = \widetilde{V}_1 \widetilde{L}$ *and* $\Lambda(\widetilde{L}) \cap (\Lambda(\widetilde{A}) \setminus \Lambda(\widetilde{L})) = \emptyset$.

We see from Proposition 4.8 that the perturbation of (V_1, L) is bounded by

$$\begin{cases} \|\widetilde{V}_1 - V_1\| = \|V_2 S\| \le \frac{2\|V_2\|\|E\|}{sep(L+F_{11}, M+F_{22})} = 2\|V_2\|\big\|\widetilde{\mathbb{S}}^{-1}\big\|\|E\|, \quad \text{and} \\ \|\widetilde{L} - L\| = \|F_{11} + F_{12}S\| \le \|W_1^H E\| + 2\big\|\widetilde{\mathbb{S}}^{-1}\big\|\|W_1^H E V_2\|\|E\| \end{cases}, \tag{4.8}$$

where $\widetilde{\mathbb{S}} : Q \to Q(L + F_{11}) - (M + F_{22})Q$ is a perturbed variant of the Sylvester operator $\mathbb{S} : Q \to QL - MQ$. We assume that the perturbation is small enough so that $\widetilde{\mathbb{S}}$ is nonsingular. Later we will compare our perturbation results for the nonlinear case with these bounds.

To begin the perturbation analysis, first note that the error estimate of the approximate invariant pair (X, G) given in Theorem 4.6 can be used for this purpose. In fact, the invariant pair (V, L) of the original problem (2.1) is an approximate invariant pair of a slightly perturbed nonlinear eigenproblem

$$\widetilde{T}(\lambda) \equiv \sum_{j=1}^{m} f_j(\lambda)(A_j + \delta A_j) = T(\lambda) + E(\lambda). \tag{4.9}$$

Here, we assume that small perturbations arise in the matrices $\{A_j\}$, which in many applications come from the discretization of differential equations; $\{f_j\}$ are often fixed functions, e.g., standard elementary or special functions, that are not subject to perturbations. To derive the perturbation analysis, consider the operators

$$(4.10)\quad \left\{ \begin{array}{l} \widetilde{\mathbb{T}} : (X,G) \to \sum_{j=1}^{m}(A_j+\delta A_j)Xf_j(G) = \mathbb{T}(X,G)+\mathbb{E}(X,G) \\ \mathbb{V} : (X,G) \to W^H U_\ell(X,G) - I_k \end{array} \right. \quad \text{(see (2.7))}\ ,$$

where $\mathbb{E}(X,G) = \sum_{j=1}^{m} \delta A_j X f_j(G)$, and the Fréchet derivative of $\widetilde{\mathbb{T}}$

$$(4.11)\qquad \begin{aligned} \mathbb{D}\widetilde{\mathbb{T}}_{(X,G)}\ &:\ (\Delta X, \Delta G) \to \mathbb{D}\mathbb{T}_{(X,G)}(\Delta X,\Delta G) + \mathbb{D}\mathbb{E}_{(X,G)}(\Delta X,\Delta G) \\ &= \mathbb{D}\mathbb{T}_{(X,G)}(\Delta X,\Delta G) + \mathbb{E}(\Delta X, G) + \sum_{j=1}^{m} \delta A_j X \mathbb{D}f_{j(G)}(\Delta G). \end{aligned}$$

One can see that $\mathbb{D}\widetilde{\mathbb{T}}$ is close to $\mathbb{D}\mathbb{T}$ if $\{\|\delta A_j\|\}$ are small. In fact, we have

$$(4.12)\qquad \begin{aligned} &\|\mathbb{D}\widetilde{\mathbb{T}}_{(X,G)}(\Delta X,\Delta G) - \mathbb{D}\mathbb{T}_{(X,G)}(\Delta X,\Delta G)\| \\ &\le \left\| \mathbb{E}(\Delta X, G) + \sum_{j=1}^{m} \delta A_j X \mathbb{D}f_{j(G)}(\Delta G) \right\| \\ &\le \sum_{j=1}^{m} \|\delta A_j\| \|\Delta X f_j(G) + X\mathbb{D}f_{j(G)}(\Delta G)\| \\ &\le \sum_{j=1}^{m} \|\delta A_j\| \left(\|f_j(G)\|\|\Delta X\| + \|X\|\|\mathbb{D}f_{j(G)}\|\|\Delta G\| \right) \\ &\le \sum_{j=1}^{m} \|\delta A_j\| \left(\|f_j(G)\| + \|X\|\|\mathbb{D}f_{j(G)}\| \right) \|(\Delta X,\Delta G)\|. \end{aligned}$$

The Fréchet derivative of the perturbed problem is therefore

$$(4.13)\qquad \widetilde{\mathbb{L}}_{(X,G)} : (\Delta X, \Delta G) \to \left(\mathbb{D}\widetilde{\mathbb{T}}_{(X,G)}(\Delta X,\Delta G), \mathbb{D}\mathbb{V}_{(X,G)}(\Delta X,\Delta G) \right),$$

which, from (4.12), satisfies

$$(4.14)\qquad \left\| \widetilde{\mathbb{L}}_{(X,G)} - \mathbb{L}_{(X,G)} \right\| \le \sum_{j=1}^{m} \|\delta A_j\| (\|f_j(G)\| + \|X\|\|\mathbb{D}f_{j(G)}\|).$$

To develop the perturbation analysis of a simple invariant pair (V, L), it suffices to show that 1) $\widetilde{\mathbb{L}}_{(V,L)}$ is nonsingular, 2) $\widetilde{\mathbb{L}}$ is Lipschitz continuous, and 3) $\|\widetilde{\mathbb{T}}(V,L)\|$ is small enough. Then the existence and uniqueness of a nearby invariant pair $(\widetilde{V}, \widetilde{L})$ of the perturbed problem can be established by the Newton-Kantorovich theorem. Conditions 1) and 3) hold if the perturbations $\{\|\delta A_j\|\}$ $(j = 1, 2, \ldots, m)$ are small. Specifically, note that $\mathbb{L}_{(V,L)}$ is nonsingular (see Theorem 2.4), and the eigenvalues of linear operators in a finite dimensional space change continuously under perturbation; see, e.g., [28], [30]. Therefore, if $\{\|\delta A_j\|\}$ are small enough, $\left\|\widetilde{\mathbb{L}}_{(V,L)} - \mathbb{L}_{(V,L)}\right\|$ is small, and the nonsingularity of $\widetilde{\mathbb{L}}_{(V,L)}$ can be guaranteed; in addition,

$$\left\|\widetilde{\mathbb{T}}(V,L)\right\| = \|\mathbb{E}(V,L)\| \le \sum_{j=1}^{m} \|\delta A_j\| \|V f_j(L)\|$$

is also small. The Lipschitz continuity of $\widetilde{\mathbb{L}}$ can be shown the same way as we did for $\mathbb{L}$ in Lemma 4.5. In summary, the perturbation analysis of a simple invariant pair (V, L) of the nonlinear eigenvalue problem (2.1) is given in the following theorem.

THEOREM 4.9. *Let $(V, L) \in \mathbb{C}_\Gamma^{n\times k} \times \mathbb{C}_\Omega^{k\times k}$ be a simple invariant pair of* (2.1), *where $\mathbb{C}_\Gamma^{n\times k}$ is bounded and convex, and $\mathbb{C}_\Omega^{k\times k}$ is open and convex with bounded Ω. For the perturbed nonlinear eigenproblem* (4.9), *suppose that the Fréchet derivative $\widetilde{\mathbb{L}}$ defined in* (4.13) *is nonsingular at (V, L), and $\kappa = \|\widetilde{\mathbb{L}}_{(V,L)}^{-1}\|$ is finite, and there exists $\gamma > 0$ such that $\|\widetilde{\mathbb{L}}_{(X_1,G_1)} - \widetilde{\mathbb{L}}_{(X_2,G_2)}\| \le \gamma \|(X_1 - X_2, G_1 - G_2)\|$ for all $(X_1, G_1), (X_2, G_2) \in \mathbb{C}_\Gamma^{n\times k} \times \mathbb{C}_\Omega^{k\times k}$. Suppose that $\{\|\delta A_j\|\}$ are small, such that $\delta = \|\widetilde{\mathbb{L}}_{(V,L)}^{-1}(\widetilde{\mathbb{T}}(V, L), 0)\|$ satisfies $h \equiv 2\kappa\gamma\delta \le 1$, and that $B((V, L), \frac{2\delta}{1+\sqrt{1-h}}) \subset \mathbb{C}_\Gamma^{n\times k} \times \mathbb{C}_\Omega^{k\times k}$, then there is a unique invariant pair $(\widetilde{V}, \widetilde{L})$ of* (4.9) *in $B((V, L), \frac{1+\sqrt{1-h}}{\kappa\gamma}) \cap \left(\mathbb{C}_\Gamma^{n\times k} \times \mathbb{C}_\Omega^{k\times k}\right)$ (if $h < 1$) or in $\overline{B((V, L), \frac{1}{\kappa\gamma})}$ (if $h = 1$) such that $\|(\widetilde{V} - V, \widetilde{L} - L)\| \le \frac{2\delta}{1+\sqrt{1-h}}$.*

Similar to the approximation error analysis given in the previous section, the perturbation of the invariant pair is bounded by $d_s \equiv \frac{2\delta}{1+\sqrt{1-h}}$, which satisfies

$$\delta \le d_s \le 2\delta = 2\|\widetilde{\mathbb{L}}_{(V,L)}^{-1}(\widetilde{\mathbb{T}}(V, L), 0)\| \le 2\|\widetilde{\mathbb{L}}_{(V,L)}^{-1}\|\|\mathbb{E}(V, L)\|. \tag{4.15}$$

This bound shows that $2\|\widetilde{\mathbb{L}}_{(V,L)}^{-1}\|$ is the condition number of a simple invariant pair under perturbation of $\{A_j\}$ of the problem (2.1). From (4.8), we see that the condition number of the simple eigenspace V_1 of the matrix A is $2\|V_2\|\|\widetilde{\mathbb{S}}^{-1}\|$. Both condition numbers are proportional to the norm of an inverse perturbed linear operator. Recall that the reciprocal of this norm describes the separation between the desired spectrum $\Lambda(\widetilde{L})$ and the rest of the spectrum of the perturbed eigenvalue problem. The smaller the separation is, the larger the condition number we have.

It is worth noting that the bound in Theorem 4.9 is very similar to the one presented in [2, Theorem 8] for polynomial eigenproblems. There are, nevertheless, several minor differences. Specifically, the bound in [2]: 1) includes an orthogonal projector which projects out the component of the perturbation that lies in the manifold of all invariant pairs equivalent to (V, L); 2) it uses $\mathbb{L}_{(V,L)}^{-1}$ instead of the perturbed variant $\widetilde{\mathbb{L}}_{(V,L)}^{-1}$; and 3) it includes a $\mathcal{O}(\|\widetilde{\mathbb{T}}(\cdot) - \mathbb{T}(\cdot)\|^2)$ term, because it is based on a first-order perturbation analysis. In spite of these differences, both bounds show the similar idea: the perturbation of simple invariant pairs are proportional to the perturbation of the problem data, and condition number is the norm of the inverse Fréchet derivative $\mathbb{L}_{(V,L)}^{-1}$ or its perturbed variant.

4.3. Subspace projection of $T(\cdot)$ and the block Rayleigh functional. In this section, we investigate the projection (restriction) of the nonlinear eigenproblem $T(\cdot)$ defined in (2.1) onto an approximate eigenspace. This projection is the block version of the nonlinear Rayleigh functional [23].

Rayleigh functionals are generalizations of Rayleigh quotients of linear eigenvalue problems to the nonlinear case. Consider the generalized linear eigenvalue problem $Av = \lambda Bv$, i.e., $T(\lambda)v = (\lambda B - A)v = 0$, with a given approximate eigenvector $x \approx v$. One can choose an auxiliary vector y such that $y^H Bx \neq 0$, and define the Rayleigh quotient as $\rho(y, x) = (y^H Ax)/(y^H Bx)$, which is in fact the solution of $y^H T(\rho)x = 0$. Similarly, for the nonlinear eigenproblem $T(\cdot)$ defined in (2.1), the Rayleigh functional $\rho(y, x)$ is defined as the solution of $y^H T(\rho)x = 0$ that satisfies $y^H T'(\rho)x \neq 0$; see [23].

The Rayleigh quotient and the Rayleigh functional can be considered as the projection of the nonlinear eigenproblem $T(\cdot)$ onto the one-dimensional right space span$\{x\}$ and left space span$\{y\}$. In particular, if $x = v$, then $\rho(y, v) = \lambda$ is the corresponding eigenvalue; see [23, Theorem 5]. This is consistent with the fact that the projection of a square matrix A onto an invariant subspace V of dimension k is a matrix $L \in \mathbb{C}^{k\times k}$ whose eigenvalues are identical to those of A corresponding to V. The projection of A onto an approximate invariant subspace is called the Rayleigh-Ritz projection and is often used to obtain eigenvalue approximations called Ritz values.

Consider an exact invariant pair (V, L) and a corresponding approximate pair (X, G), respectively, of the nonlinear nonlinear eigenproblem $T(\cdot)$. The idea discussed above can be used to study the projection of $T(\cdot)$ onto the right space span$\{X\}$ and left space span$\{Y\}$. For some given $Y, X \in \mathbb{C}^{n\times k}$, define the operator

$$\mathbb{P}^{(Y,X)} : G \to \sum_{j=1}^{m} Y^H A_j X f_j(G).$$

Note that $\mathbb{P}^{(Y,V)}(L) = Y^H \mathbb{T}(V, L) = 0$, because (V, L) is an invariant pair. Therefore, if X is sufficiently close to V, then

$$\begin{aligned} \|\mathbb{P}^{(Y,X)}(L)\| &= \left\| \sum_{j=1}^{m} Y^H A_j X f_j(L) \right\| \\ &= \left\| \sum_{j=1}^{m} Y^H A_j (X - V) f_j(L) \right\| \le \|X - V\| \sum_{j=1}^{m} \|Y^H A_j\| \|f_j(L)\| \end{aligned}$$

is also small.

Following the lines of the proof of Lemma 4.5, we can show that $\mathbb{DP}^{(Y,X)}_{(L)}$ is Lipschitz continuous if the Fréchet derivatives $\{\mathbb{D}f_j\}$ are Lipschitz continuous. Assume that for an approximate invariant pair (X, G), Y is chosen such that the Fréchet derivative

$$\mathbb{DP}^{(Y,X)}_{(L)} : \Delta G \to \sum_{j=1}^{m} Y^H A_j X \mathbb{D}f_{j(L)}(\Delta G) \tag{4.16}$$

is nonsingular. This assumption is a block generalization of $y^H T'(\lambda) x \neq 0$, which is needed to make sure that the Rayleigh functional $\rho(x, y)$ is well-defined; see [23]. This condition holds in general for the two-sided scalar Rayleigh functional approximating non-defective eigenvalues λ, if x and y are close to appropriate right and left eigenvectors, respectively. Specifically, as we will discuss shortly, one can always choose a right eigenvector v and a left eigenvector w corresponding to a non-defective λ, such that $w^H T'(\lambda) v = 1$. Therefore, $y^H T'(\lambda) x \neq 0$ if x and y are sufficiently close v and w, respectively. For the block case, however, we do not have a complete understanding of the conditions under which the the Fréchet derivative $\mathbb{DP}^{(Y,X)}_{(L)}$ is nonsingular.

In the following theorem, we summarize some properties of a block Rayleigh functional, which are obtained by applying the Newton-Kantorovich Theorem to $\mathbb{P}^{(Y,X)}$.

THEOREM 4.10. *Let $(V, L), (X, G) \in \mathbb{C}^{n\times k}_{\Gamma} \times \mathbb{C}^{k\times k}_{\Omega}$ be an exact and a corresponding approximate minimal invariant pair of* (2.1)*, respectively, where $\mathbb{C}^{n\times k}_{\Gamma}$ is bounded and convex, and $\mathbb{C}^{k\times k}_{\Omega}$ is open and convex with bounded Ω. Suppose $Y \in \mathbb{C}^{n\times k}$ is such that the Fréchet derivative $\mathbb{DP}^{(Y,X)}_{(L)}$ defined in* (4.16) *is nonsingular, and $\kappa = \left\|(\mathbb{DP}^{(Y,X)}_{(L)})^{-1}\right\|$*

is finite, and there exists $\gamma > 0$ *such that* $\left\|\mathbb{D}\mathbb{P}^{(Y,X)}_{(L_1)} - \mathbb{D}\mathbb{P}^{(Y,X)}_{(L_2)}\right\| \leq \gamma\|L_1 - L_2\|$ *for all* $L_1, L_2 \in \mathbb{C}^{k\times k}_\Omega$*. Suppose that* X *is close to* V*, such that* $\delta = \left\|(\mathbb{D}\mathbb{P}^{(Y,X)}_{(L)})^{-1}\mathbb{P}_{(Y,X)}(L)\right\|$ *satisfies* $h \equiv 2\kappa\gamma\delta \leq 1$*, and* $B(L, \frac{2\delta}{1+\sqrt{1-h}}) \subset \mathbb{C}^{k\times k}_\Omega$*, then there is a unique block Rayleigh functional* Q *satisfying* $\mathbb{P}^{(Y,X)}(Q) = Y^H\mathbb{T}(X,Q) = 0$ *in* $B(L, \frac{1+\sqrt{1-h}}{\kappa\gamma}) \cap \mathbb{C}^{k\times k}_\Omega$ (if $h < 1$) *or in* $\overline{B(L, \frac{1}{\kappa\gamma})}$ (if $h = 1$) *such that* $\|Q - L\| \leq \frac{2\delta}{1+\sqrt{1-h}}$*.*

Theorem 4.10 gives an approximation error estimate of the block Rayleigh functional Q, namely, $\|Q - L\| \leq d_s = \frac{2\delta}{1+\sqrt{1-h}}$, which satisfies

$$\delta \leq d_s \leq 2\delta = 2\left\|(\mathbb{D}\mathbb{P}^{(Y,X)}_{(L)})^{-1}\mathbb{P}_{(Y,X)}(L)\right\| \leq 2\left\|(\mathbb{D}\mathbb{P}^{(Y,X)}_{(L)})^{-1}\right\|\|\mathbb{P}^{(Y,X)}(L)\|. \tag{4.17}$$

From (4.17), we can show that for the special case where both the left and the right spaces are of one dimension ($k = 1$), the *scalar* Rayleigh functional studied in [23] may provide an eigenvalue approximation of higher order accuracy. In fact, let (λ, v) and (λ, w) be a right and a left eigenpair of the problem (2.1), respectively, such that $w^H T(\lambda) = 0$, $T(\lambda)v = 0$ and $\|v\| = \|w\| = 1$. Consider $x = \cos\alpha v + \sin\alpha v_\perp$ and $y = \cos\beta w + \sin\beta w_\perp$, where $\alpha, \beta < \frac{\pi}{2}$, and $v_\perp \perp v$ and $w_\perp \perp w$ are unit vectors such that $\|x\| = \|y\| = 1$. Then, noting that $X = x$, $Y = y$ and $L = \lambda$, we have

$$\begin{aligned} \|\mathbb{P}^{(Y,X)}(L)\| &= \left|\sum_{j=1}^m y^H A_j x f_j(\lambda)\right| \\ &= \left|\sum_{j=1}^m (\overline{\cos\beta} w^H + \overline{\sin\beta} w_\perp^H) A_j (\cos\alpha v + \sin\alpha v_\perp) f_j(\lambda)\right| \\ &\leq \left|\overline{\cos\beta}\big(w^H T(\lambda)\big)(\cos\alpha v + \sin\alpha v_\perp)\right| + \left|\overline{\sin\beta}\Big(\sum_{j=1}^m w_\perp^H A_j f_j(\lambda)\Big)(\cos\alpha v + \sin\alpha v_\perp)\right| \\ &= |\sin\beta|\left|\cos\alpha w_\perp^H\big(T(\lambda)v\big) + \sin\alpha\sum_{j=1}^m w_\perp^H A_j f_j(\lambda) v_\perp\right| \\ &= |w_\perp^H T(\lambda) v_\perp||\sin\alpha\sin\beta| \leq \|T(\lambda)\||\sin\alpha\sin\beta|\ , \end{aligned} \tag{4.18}$$

and for small α and β

$$\begin{aligned} \left\|(\mathbb{D}\mathbb{P}^{(Y,X)}_{(L)})^{-1}\right\| &= \left|\sum_{j=1}^m (y^H A_j x) f_j'(\lambda)\right|^{-1} = |y^H T'(\lambda) x|^{-1} \\ &= \Big|\overline{\cos\beta}\cos\alpha w^H T'(\lambda) v + \overline{\cos\beta}\sin\alpha w^H T'(\lambda) v_\perp \\ &\qquad + \overline{\sin\beta}\cos\alpha w_\perp^H T'(\lambda) v + \overline{\sin\beta}\sin\alpha w_\perp^H T'(\lambda) v_\perp^H\Big|^{-1} \\ &\leq \big(|\cos\alpha\cos\beta||w^H T'(\lambda) v| - (|\sin\alpha\cos\beta| + |\cos\alpha\sin\beta| + |\sin\alpha\sin\beta|)\|T'(\lambda)\|\big)^{-1}. \end{aligned}$$

From (4.17), for small α and β, the error estimate of the scalar Rayleigh functional as an approximation of λ is

$$\begin{aligned} |q(y,x) - \lambda| &\leq \frac{2\|T(\lambda)\||\sin\alpha\sin\beta|}{|y^H T'(\lambda) x|} \\ &\leq \frac{2\|T(\lambda)\||\tan\alpha\tan\beta|}{|w^H T'(\lambda) v| - (|\tan\alpha| + |\tan\beta| + |\tan\alpha\tan\beta|)\|T'(\lambda)\|}\ . \end{aligned} \tag{4.19}$$

For the linear eigenproblem $Av - v\lambda = 0$, exactly this bound has been derived in [22, Proposition 5]. For nonlinear eigenproblems, it is shown in [23, Remark 3.9] that the bound can be improved to $|q(y,x) - \lambda| \leq \dfrac{\|T(\lambda)\| |\tan\alpha\tan\beta|}{|w^H T'(\lambda)v|(1 - \mathcal{O}(\tan\alpha + \tan\beta))}$.

Therefore, if $w^H T'(\lambda)v \neq 0$, the two-sided scalar Rayleigh functional is an eigenvalue approximation of *second order* accuracy for small α and β; if $w^H T'(\lambda)v = 0$, then the last expression in (4.19) indicates that only *first order* accuracy can be achieved. In fact, whether $w^H T'(\lambda)v = 0$ basically depends on if λ is a defective eigenvalue. Specifically, assume that the geometric multiplicity of λ is g, and $\{\varphi_1, \varphi_2, \ldots, \varphi_g\}$ and $\{\psi_1, \psi_2, \ldots, \psi_g\}$ are corresponding right and left eigenvectors, respectively. Then it is shown in [11, Theorem A.10.2] that the two sets of eigenvectors can be chosen such that $\psi_i^H T'(\lambda)\varphi_j = \delta_{ij}$ $(i, j = 1, 2, \ldots, g)$ for non-defective (simple or semisimple) λ. For defective λ, however, we always have $\psi_i^H T'(\lambda)\varphi_j = 0$. It follows that second order accuracy of the two-sided scalar Rayleigh functional can only be achieved for non-defective eigenvalues.

We find that the above result on second order accuracy in eigenvalue approximation in the scalar case can be extended to the two-sided *block* Rayleigh functional for non-defective eigenvalues. The result is summarized in the following theorem.

THEOREM 4.11. *Let (V, L) and (X, G) be an exact and a corresponding approximate invariant pair of (2.1), respectively. Let $Y \in \mathbb{C}^{n\times k}$ be such that* $\mathrm{range}(Y)$ *is close to the span of the corresponding left eigenvectors. Assume that the conditions of Theorem 4.10 are satisfied, so that there exists a unique block Rayleigh functional Q satisfying $\|Q - L\| \leq \frac{2\delta}{1+\sqrt{1-h}} \leq 2\delta$. Let λ be an eigenvalue of $T(\cdot)$ and L, and v and w be a corresponding right and a left eigenvector. Suppose that there exist $x \in \mathrm{range}(X)$ and $y \in \mathrm{range}(Y)$ such that $\alpha = \angle(x, v)$ and $\beta = \angle(y, w)$ are sufficiently small. If λ is a simple eigenvalue of $T(\cdot)$, or if λ is semi-simple and $w^H T'(\lambda)v \neq 0$, then the block Rayleigh functional Q has an eigenvalue $\tilde\lambda$ such that $|\tilde\lambda - \lambda| \leq \mathcal{O}(\sin\alpha\sin\beta)$. If λ is a defective eigenvalue of $T(\cdot)$, then Q has an eigenvalue $\tilde\lambda$ such that $|\tilde\lambda - \lambda| \leq \mathcal{O}(\min(\alpha, \beta))$.*

The proof of Theorem 4.11 is given in Appendix A.

5. Structure and norm estimate of Fréchet derivatives. Let (V, L) be a simple invariant pair of (2.1), and (X, G) be a corresponding approximate invariant pair. In Section 4, we showed that the norms of the inverse Fréchet derivatives $\mathbb{L}^{-1}_{(X,G)}$ and $\widetilde{\mathbb{L}}^{-1}_{(V,L)}$, play an important role in the analysis of approximation errors and perturbations of invariant pairs; see (4.6) and (4.15). In this section, we analyze the algebraic structure of the Fréchet derivative $\mathbb{L}_{(V,L)}$, and we briefly discuss an norm estimate of the inverse derivative $\mathbb{L}^{-1}_{(V,L)}$. Since both $\mathbb{L}^{-1}_{(X,G)}$ and $\widetilde{\mathbb{L}}^{-1}_{(V,L)}$ are perturbed variants of $\mathbb{L}^{-1}_{(V,L)}$, a norm estimate of the latter can be used as an estimate of the former, and thus it may give a quantitative description of conditioning and sensitivity of invariant pairs.

Before we present the norm estimate of $\mathbb{L}^{-1}_{(V,L)}$, recall that the expression of the Fréchet derivative from (2.8) and (2.9) is

$$\begin{aligned}(5.1)\qquad \mathbb{L}_{(V,L)} &: (\Delta X, \Delta G) \to \big(\mathbb{DT}_{(V,L)}(\Delta X, \Delta G), \mathbb{DV}_{(V,L)}(\Delta X, \Delta G)\big) \\ &= \Big(\mathbb{T}(\Delta X, L) + \sum_{j=1}^{m} A_j V \mathbb{D} f_{j(L)}(\Delta G),\ \sum_{j=0}^{\ell-1} W_j^H \Delta X L^j + \sum_{j=1}^{\ell-1} W_j^H V[\mathbb{D}L^j](\Delta G)\Big),\end{aligned}$$

which is a linear mapping on $\mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$. Since a linear mapping on a finite dimensional linear space can be represented by a matrix, the structure of $\mathbb{L}_{(V,L)}$ can be understood by studying the matrix representation of the Fréchet derivative.

THEOREM 5.1. *Let* (V, L) *be a simple invariant pair of* (2.1) *and* $\mathbb{L}_{(V,L)}$ *be the corresponding Fréchet derivative defined in* (5.1). *Let* $\begin{bmatrix} H & M \\ N & K \end{bmatrix}$ *be the matrix representation of* $\mathbb{L}_{(V,L)}$*, where* $H \in \mathbb{C}^{nk\times nk}$*,* $M \in \mathbb{C}^{nk\times k^2}$*,* $N \in \mathbb{C}^{k^2\times nk}$ *and* $K \in \mathbb{C}^{k^2\times k^2}$*, such that* $vec\left(\mathbb{L}_{(V,L)}(\Delta X, \Delta G)\right) = \begin{bmatrix} H & M \\ N & K \end{bmatrix}\begin{bmatrix} vec(\Delta X) \\ vec(\Delta G) \end{bmatrix}$ *for all* $(\Delta X, \Delta G) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$*. Then*

$$1 \le r \equiv \dim(\ker(H)) \le k^2.$$

Here, $r = 1$ *if and only if* L *has only one distinct eigenvalue and is similar to a single Jordan block of order* k*;* $r = k$ *if* L *has* k *distinct simple eigenvalues;* $r = k^2$ *if and only if* L *has only one distinct eigenvalue that is semi-simple. Let* $H = Y_a \begin{bmatrix} \Sigma_{11} & 0 \\ 0 & 0 \end{bmatrix} Y_b^H$ *be the singular value decomposition of* H*, where* $\Sigma_{11} \in \mathbb{C}^{(nk-r)\times(nk-r)}$ *contains all the nonzero singular values of* H*. Define*

$$F_* \equiv \begin{bmatrix} Y_a^H & 0 \\ 0 & I_{k^2} \end{bmatrix}\begin{bmatrix} H & M \\ N & K \end{bmatrix}\begin{bmatrix} Y_b & 0 \\ 0 & I_{k^2} \end{bmatrix} = \begin{bmatrix} Y_a^H H Y_b & Y_a^H M \\ N Y_b & K \end{bmatrix} = \begin{bmatrix} \Sigma_{11} & 0 & M_{13} \\ 0 & 0 & M_{23} \\ N_{31}^H & N_{32}^H & K \end{bmatrix},$$

where $M_{13} \in \mathbb{C}^{(nk-r)\times k^2}$*,* $M_{23} \in \mathbb{C}^{r\times k^2}$*,* $N_{31}^H \in \mathbb{C}^{k^2\times(nk-r)}$*,* $N_{32}^H \in \mathbb{C}^{k^2\times r}$*. If* F_* *is nonsingular, then* F_*^{-1} *has the following* 3×3 *block form*

$$\begin{bmatrix} \Sigma_{11}^{-1} - \Sigma_{11}^{-1} M_{13} Q_3^{-1} Q_0 & \Sigma_{11}^{-1} M_{13} Q_3^{-1} N_{32}^H & -\Sigma_{11}^{-1} M_{13} Q_3^{-1}\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) \\ -(N_{32}^H)_L^{-1} N_{31}^H \Sigma_{11}^{-1} - Q_2 Q_3^{-1} Q_0 & I + Q_2 Q_3^{-1} N_{32}^H & (N_{32}^H)_L^{-1} - Q_2 Q_3^{-1}\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) \\ Q_3^{-1} Q_0 & -Q_3^{-1} N_{32}^H & Q_3^{-1}\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) \end{bmatrix},$$

where $(N_{32}^H)_L^{-1} = (N_{32} N_{32}^H)^{-1} N_{32} \in \mathbb{C}^{r\times k^2}$ *is the left inverse of* N_{32}^H*, and*

$$\begin{aligned} Q_0 &= -\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) N_{31}^H \Sigma_{11}^{-1} \in \mathbb{C}^{k^2\times(nk-r)}, \\ Q_1 &= K_{33} - N_{31}^H \Sigma_{11}^{-1} M_{13} \in \mathbb{C}^{k^2\times k^2}, \\ Q_2 &= M_{23} + (N_{32}^H)_L^{-1} Q_1 \in \mathbb{C}^{r\times k^2}, \\ Q_3 &= Q_1 - N_{32}^H Q_2 = \left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) Q_1 - N_{32}^H M_{23} \in \mathbb{C}^{k^2\times k^2}. \end{aligned}$$

The proof of this theorem is given in Appendix B.

REMARK 5.2. It follows from Theorem 5.1 that, given the block matrix representation of $\mathbb{L}_{(V,L)}$, we may define the norm of the inverse derivative $\mathbb{L}_{(V,L)}^{-1}$ as, for example,

$$\|\mathbb{L}_{(V,L)}^{-1}\| \equiv \left\| \begin{bmatrix} H & M \\ N & K \end{bmatrix}^{-1} \right\|_2 = \|F_*^{-1}\|_2,$$

and thus an upper bound of this norm can be obtained by summing up the norm of each block of the matrix form of F_*^{-1}. In particular, we see from this block matrix that a large $\left\|\Sigma_{11}^{-1}\right\|_2$ indicates that $\left\|F_*^{-1}\right\|_2$ is large. For example, in the special case where L has only one distinct semi-simple eigenvalue such that $\dim(\ker(H)) = k^2$, this block matrix can be simplified, and one can follow [21, Lemma 4.5] and show that

$$\left\|F_*^{-1}\right\|_2 \leq \left\|\Sigma_{11}^{-1}\right\|_2 \left(1 + \left\|(N_{32}^H)^{-1}N_{31}^H\right\|_2\right)\left(1 + \left\|M_{13}M_{23}^{-1}\right\|_2\right) + \left\|(N_{32}^H)^{-1}KM_{23}^{-1}\right\|_2 + \left\|M_{23}^{-1}\right\|_2 + \left\|(N_{32}^H)^{-1}\right\|_2. \tag{5.2}$$

Here, the upper bound depends linearly on $\left\|\Sigma_{11}^{-1}\right\|_2$. In the scalar case ($k = r = 1$), λ is simple, and $\begin{bmatrix} H & M \\ N & K \end{bmatrix} = \begin{bmatrix} T(\lambda) & T'(\lambda)v \\ \frac{v^H}{\|v\|_2^2} & 0 \end{bmatrix}$, $M_{23} = e_n^T Y_a^H T'(\lambda)v = \frac{w^H}{\|w\|_2}T'(\lambda)v = \frac{1}{\|w\|_2} \neq 0$, and $N_{32}^H = \frac{v^H}{\|v\|_2^2}Y_b e_n = \frac{v^H}{\|v\|_2^2}\frac{v}{\|v\|_2} = \frac{1}{\|v\|_2} \neq 0$. Therefore the last three terms in the upper bound of (5.2) are finite, and they bear no connections to the separation between λ, the eigenvalue of interest, and the rest of the spectrum. In the block case where λ is semi-simple, we have no proof, but we conjecture that the same observation still holds for these terms.

Note that $\left\|\Sigma_{11}^{-1}\right\|_2$ is the reciprocal of the smallest nonzero singular value of H, i.e., the matrix representation of the functional $\Delta X \to \mathbb{T}(\Delta X, L)$. In the special case when $k = 1$ and $L = \lambda$, this functional degenerates to the matrix $T(\lambda)$, and its smallest nonzero singular value is relevant to estimate the separation between λ and the rest of the spectrum of $T(\cdot)$. A very small singular value indicates that the separation is small, though the inverse may not be true, for example, in certain cases where λ is highly ill-conditioned. By analogy, the smallest nonzero singular value of H may also be useful to estimate the separation between $\Lambda(L) \subset \Lambda(T(\cdot))$ and $\Lambda(T(\cdot)) \setminus \Lambda(L)$. If the estimate of $\left\|\mathbb{L}_{(V,L)}^{-1}\right\|$ is a reasonable estimate of $\left\|\mathbb{L}_{(X,G)}^{-1}\right\|$ and $\left\|\widetilde{\mathbb{L}}_{(V,L)}^{-1}\right\|$, then large separation between the desired spectrum and the rest of the spectrum is desirable for numerical algorithms to compute the wanted invariant pairs. In this case, an approximate invariant pair with small eigenresidual norm is indeed close to the exact invariant pair, and the exact invariant pair is not very sensitive to perturbations.

We conclude this section by discussing an estimate of $\left\|\mathbb{L}_{(X,G)}^{-1}\right\|$ and $\left\|\widetilde{\mathbb{L}}_{(V,L)}^{-1}\right\|$, i.e., the condition numbers in the quantification of approximation errors and perturbations of invariant pairs; see Theorems 4.6 and 4.9. For example, following the treatment of $\mathbb{L}_{(V,L)}$ in Appendix B, we have $\begin{bmatrix} \widetilde{H} & \widetilde{M} \\ \widetilde{N} & \widetilde{K} \end{bmatrix}$ as the matrix representation of $\widetilde{\mathbb{L}}_{(V,L)}$. Define $\widetilde{F} = \begin{bmatrix} Y_a^H & 0 \\ 0 & I_{k^2} \end{bmatrix}\begin{bmatrix} \widetilde{H} & \widetilde{M} \\ \widetilde{N} & \widetilde{K} \end{bmatrix}\begin{bmatrix} Y_b & 0 \\ 0 & I_{k^2} \end{bmatrix}$, as F_* is defined in (B.3). Then $\widetilde{F} \to F_*$ if the perturbation $\{\delta A_j\} \to 0$. Suppose that the perturbation is sufficiently small, such that $\widetilde{F}$ is close enough to F_*. Then there is $\eta < 1$ such that

$$\left\|F_*^{-1}(\widetilde{F} - F_*)\right\| = \left\|I - F_*^{-1}\widetilde{F}\right\| \leq \eta. \tag{5.3}$$

Therefore $\lim_{k\to\infty}\left(I - F_*^{-1}\widetilde{F}\right)^k = 0$, $I - (I - F_*^{-1}\widetilde{F}) = F_*^{-1}\widetilde{F}$ is nonsingular (see, e.g., [26, Theorem 4.20]), and $\widetilde{F}$ is nonsingular. From (5.3), we have in the *2-norm*

$$\begin{aligned} \left\|\widetilde{F}^{-1}F_*\right\| - 1 &\leq \left\|\widetilde{F}^{-1}F_* - I\right\| = \left\|\left(I - F_*^{-1}\widetilde{F}\right)\widetilde{F}^{-1}F_*\right\| \\ &\leq \left\|I - F_*^{-1}\widetilde{F}\right\|\left\|\widetilde{F}^{-1}F_*\right\| \leq \eta\left\|\widetilde{F}^{-1}F_*\right\| \\ \Rightarrow \quad \left\|\widetilde{F}^{-1}F_*\right\| &\leq (1-\eta)^{-1} \\ \Rightarrow \quad \left\|\widetilde{F}^{-1}\right\| &= \left\|\widetilde{F}^{-1}F_*F_*^{-1}\right\| \leq \left\|\widetilde{F}^{-1}F_*\right\|\left\|F_*^{-1}\right\| \leq (1-\eta)^{-1}\left\|F_*^{-1}\right\|. \end{aligned}$$

Assume that the perturbations are small such that η is not very close to 1. Then $\|\widetilde{\mathbb{L}}^{-1}_{(V,L)}\| = \|\widetilde{F}^{-1}\|$ is bounded above by a modest multiple of $\|\mathbb{L}^{-1}_{(V,L)}\| = \|F_*^{-1}\|$. The analysis can be applied verbatim to the estimate of $\|\mathbb{L}^{-1}_{(X,G)}\|$.

6. Numerical Examples. In this section, we give numerical examples to illustrate the properties of invariant pairs: 1) given a simple invariant pair (V, L) and a corresponding approximate pair (X, G), we give evidence that $\|(X - V, G - L)\|$ is proportional to the eigenresidual norm $\|\mathbb{T}(X, G)\|$; 2) for simple invariant pairs (V, L) and $(\widetilde{V}, \widetilde{L})$ of the original and the perturbed problems, we show that $\|(\widetilde{V} - V, \widetilde{L} - L)\|$ is proportional to the perturbation of $T(\cdot)$, and 3) the second order accuracy in eigenvalue approximation can be achieved by the *two-sided* block Rayleigh functional Q that approximates the non-defective eigenvalues of L .

We start with the description of the example eigenvalue problem. Consider the following nonlinear eigenproblem:

$$T(\mu) = \begin{bmatrix} \mu-\lambda_1 & & & \mu^3 & & & & \\ & \mu-\lambda_2 & & \mu^2 & & & & \\ & & \mu-\lambda_3 & \mu & & & & \\ & & & (\mu-\lambda_4)^2 & & & & \\ 5\mu & 100\mu^2 & 0 & \mu^3 & \mu+92 & & & \\ 6\mu & 99\mu^2 & 1 & \mu^3 & & \mu+90 & & \\ \vdots & \vdots & \vdots & \vdots & & & \ddots & \\ 100\mu & 5\mu^2 & 95 & \mu^3 & & & & \mu-98 \end{bmatrix}_{100\times 100}.$$

One see from the structure of $T(\mu)$ that if $\mu = \lambda_i$ $(i = 1, 2, 3, 4)$, then the top left 4×4 submatrix is singular, and so is $T(\mu)$. Therefore $\{\lambda_i\}$ are eigenvalues of this nonlinear eigenproblem. This is a cubic eigenproblem, and it can be solved by MATLAB's `polyeig` function.

6.1. Approximation errors. We begin the discussion with invariant pair approximation errors. First, consider a simple invariant pair involving three distinct simple eigenvalues $\lambda_1 = 3.02 + 0.01i$, $\lambda_2 = 3 + 0.02i$, and $\lambda_3 = 2.99 - 0.01i$. For this problem, the corresponding eigenvectors $\{v_i\}$ $(i = 1, 2, 3)$ are linearly independent. Let the invariant pair be $(V, L) = \big([v_1\ v_2\ v_3]S, S^{-1}\mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)S\big)$, where the entries of S obey the standard normal distribution. To construct a corresponding approximate invariant pair (X, G), we first introduce perturbations dV and dL, whose entries also obey the standard normal distribution. We then scale dV and dL such that $\|dV\| = \|V\|$ and $\|dL\| = \|L\|$. The approximate pair (X, G) is generated by the following command

```
err = 10^(-kk);  X = V + err*dV; G = L + err*dL;
```

where $kk = 1, 2, \ldots, 12$ specifies the magnitude of the invariant pair approximation error. Then we assign $(X, G) \leftarrow \big(X(X^HX)^{-1/2}, (X^HX)^{1/2}G(X^HX)^{-1/2}\big)$, so that the new X has orthonormal columns. This normalization is slightly different from imposing $W^HU_\ell(X, G) = I_k$ ($\ell = 1$ due to the linear independence of $\{v_1, v_2, v_3\}$) with W defined in (2.6), but it is used in the block Newton method for computing simple invariant pairs [12]. Our experience is that the choice of normalization has minimum impact on the numerical results.

In the left part of Figure 6.1, $\|(X - V, G - L)\|$, the invariant pair approximation error, is plotted against the eigenresidual norm $\|\mathbb{T}(X, G)\|$. We see from the solid line with $\Box$ marker that $\|(X - V, G - L)\|$ is proportional to $\|\mathbb{T}(X, G)\|$. In addition, we found that $\|X-V\|$ and $\|G-L\|$ are also proportional to $\|\mathbb{T}(X,G)\|$ with the same proportional factor. Theorem 4.6 shows that this factor should be inversely proportional to the separation between $\Lambda(L)$ and $\Lambda(T)\setminus\Lambda(L)$.

To see the approximation errors for invariant pairs involving degenerate eigenvalues, consider a semi-simple $\lambda_1=\lambda_2=\lambda_3=3+0.1i$, and a defective $\lambda_4=3$ with a single Jordan chain of length 2. For the semi-simple eigenvalue, we let $L=\lambda_1 I_3$ and obtain $V=[v_1\ v_2\ v_3]$ by directly computing $\ker T(\lambda_1)$. For the defective case, define $L=\begin{bmatrix}\lambda_4 & 1\\ 0 & \lambda_4\end{bmatrix}$, and let $v_1\in\ker T(\lambda_4)$ and $v_2=-T(\lambda_4)^{\dagger}T'(\lambda_4)v_1$ be the standard and the generalized eigenvectors, respectively. In both cases, (V,L) is a simple invariant pair. We then perform the same procedure done for simple eigenvalues. In the left part of Figure 6.1, we see from the dash-dot line with $\Diamond$ marker and the dashed line with $\triangle$ marker that $\|(X-V,G-L)\|$ is proportional to $\|\mathbb{T}(X,G)\|$ in the semi-simple and defective cases as well.

Remark 6.1. To make the understanding of the invariant pair approximation errors more complete, we briefly discuss the intuition for the inverse proportionality between $\|(X-V,G-L)\|$ and the separation between the desired spectrum and the rest of the spectrum (characterized by $\left\|\mathbb{L}^{-1}_{(X,G)}\right\|^{-1}$ in Theorem 4.6). Consider the simplest case where the desired invariant pair is a simple eigenpair (λ_*,v_*). Assume that there is a nearby simple eigenpair $(\lambda_\alpha,v_\alpha)$ such that $\|v_\alpha-v_*\|>\gamma_0>0$. Then (λ_*,v_α) is an approximate invariant pair with eigenresidual

$$\|T(\lambda_*)v_\alpha\|=\|T(\lambda_\alpha)v_\alpha+(\lambda_*-\lambda_\alpha)T'(\lambda_\alpha)v_\alpha+\mathcal{O}\left((\lambda_*-\lambda_\alpha)^2\right)\|=\mathcal{O}(\lambda_*-\lambda_\alpha).$$

Therefore, if λ_α is very close to λ_*, $\|T(\lambda_*)v_\alpha\|$ is small, but the separation between λ_* and the rest of the spectrum is also small. Indeed, since the physical distance between λ_* and $\Lambda(T(\cdot))\setminus\{\lambda_*\}$ is no greater than $|\lambda_*-\lambda_s|$, we may make a reasonable assumption that this separation is bounded above by $\mathcal{O}(\lambda_s-\lambda_*)$. As a result, the upper bound for $\|v_\alpha-v_*\|$ given in Theorem 4.6, namely, $\|T(\lambda_*)v_\alpha\|/\left\|\mathbb{L}^{-1}_{(v_\alpha,\lambda_*)}\right\|^{-1}$, is bounded below by a positive constant. This observation is consistent with the fact that $\|v_\alpha-v_*\|>\gamma_0>0$. In conclusion, if the desired spectrum is not well separated from the rest of the spectrum, an approximate invariant pair with a small eigenresidual norm does not guarantee an accurate eigenspace approximation.

6.2. Perturbations. To study the perturbation of simple invariant pairs, we generate a set of random matrices $\{\Delta A_j\}$, where each ΔA_j has the same sparsity pattern as A_j, and the entries of ΔA_j obey the standard normal distribution. Then $\{\Delta A_j\}$ are scaled so that $\|\Delta A_j\|=\|A_j\|$. The perturbed eigenproblem is thus defined as $\widetilde{T}(\mu)=\sum_{j=1}^m f_j(\mu)(A_j+\epsilon\Delta A_j)$, where ϵ is a small scaling factor controlling the magnitude of the perturbation.

We found that the three simple eigenvalues specified in Section 6.1 remain simple after such perturbation. Let $\{(\widetilde{\lambda}_i,\widetilde{v}_i)\}$ be the perturbed eigenpairs, $\widetilde{V}=[\widetilde{v}_1\ \widetilde{v}_2\ \widetilde{v}_3]$, and $\widetilde{L}=\mathrm{diag}(\widetilde{\lambda}_1,\widetilde{\lambda}_2,\widetilde{\lambda}_3)$. Then we let $(\widetilde{V},\widetilde{L})\leftarrow(\widetilde{V}\widetilde{S},\widetilde{S}^{-1}\widetilde{L}\widetilde{S})$, where $\widetilde{S}$ solves the least squares problem

$$\widetilde{S}=\arg\min_{S\in\mathbb{C}^{3\times 3}}\|V-\widetilde{V}\widetilde{S}\|_F.$$

Finally, we normalize $\widetilde{V}$ by letting $(\widetilde{V},\widetilde{L})\leftarrow\left(\widetilde{V}(\widetilde{V}^H\widetilde{V})^{-1/2},(\widetilde{V}^H\widetilde{V})^{1/2}\widetilde{L}(\widetilde{V}^H\widetilde{V})^{-1/2}\right)$.

In the right part of Figure 6.1, we plotted $\|(\widetilde{V}-V,\widetilde{L}-L)\|$ against the magnitude of eigenproblem perturbation ϵ. Clearly, the perturbation of (V,L) is proportional to

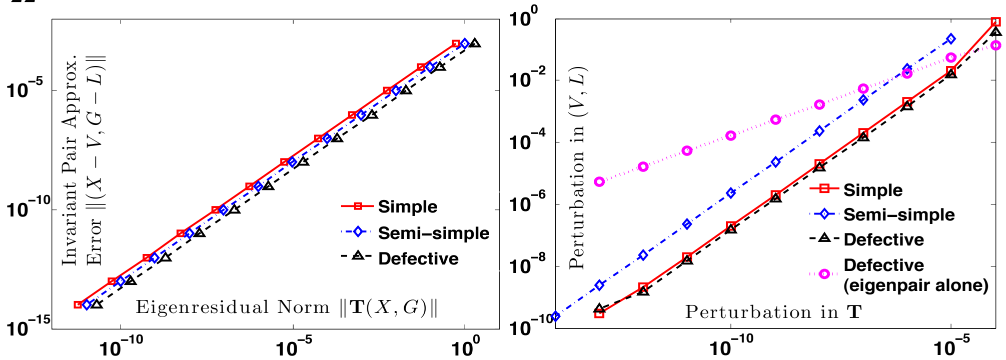

FIG. 6.1. *Approximation errors and perturbations of simple invariant pairs Left: eigenresidual norm* $\|\mathbb{T}(X,G)\|$ (x-axis) *vs. invariant pair approximation errors* $\|(X–V, G–L)\|$ (y-axis) *Right: Perturbations of* $T(\cdot)$ (x-axis) *vs. invariant pair perturbations* $\|(\widetilde{V}-V, \widetilde{L}-L)\|$ (y-axis)

the perturbation of the problem data. In addition, we also computed $\|\widetilde{V} - V\|$ and $\|\widetilde{L} - L\|$, and we found that both quantities are also proportional to ϵ.

We repeated the experiment for simple invariant pairs involving the semi-simple eigenvalue and the defective eigenvalue. Specifically, the semi-simple eigenvalue $\lambda_1 = \lambda_2 = \lambda_3 = 3 + 0.1i$ corresponds to three distinct perturbed simple eigenvalues $\widetilde{\lambda}_1, \widetilde{\lambda}_2$ and $\widetilde{\lambda}_3$; the simple invariant pair involving the defective eigenvalue is perturbed to a new invariant pair $(\widetilde{V}, \widetilde{L})$ involving two distinct simple eigenpairs $(\widetilde{\lambda}_{4a}, \widetilde{v}_{4a})$ and $(\widetilde{\lambda}_{4b}, \widetilde{v}_{4b})$. Our results again show that the perturbation of simple invariant pairs is proportional to the perturbation of the eigenproblem data. Here, it is worth pointing out that the *defective eigenpair* itself, (λ_4, v_4), is much more sensitive to perturbation than the simple invariant pair involving λ_4. We found that $\|(v_4 - v_{4a}, \lambda_4 - \lambda_{4a})\|$ and $\|(v_4 - v_{4b}, \lambda_4 - \lambda_{4b})\|$ are both proportional to $\sqrt{\epsilon}$; see the dotted line with ○ marker in the right part of Figure 6.1. This result is consistent with the well-known fact that the perturbation of an defective eigenpair is proportional to $\epsilon^{1/m}$, where m is the size of the corresponding largest Jordan block [18].

6.3. Block Rayleigh functionals. Given a minimal invariant pair (V, L) and a right eigenspace approximation $X \approx V$, Theorem 4.10 shows that the block Rayleigh functional Q satisfying $Y^H\mathbb{T}(X,Q) = \sum_{j=1}^{m} Y^H A_j X f_j(Q) = 0$ is a good approximation to L; in addition, it is shown in Theorem 4.11 that the eigenvalues of Q are approximations of second order accuracy to the non-defective eigenvalues of L, if Y contains good approximations to the corresponding left eigenvectors.

We perform numerical experiments to illustrate the above results. Consider again the simple eigenpairs (λ_i, v_i) $(i = 1, 2, 3)$ used in Sections 6.1 and 6.2. Let $\{w_i\}$ be the corresponding unit left eigenvectors, $V = [v_1\ v_2\ v_3]S$, $W = [w_1\ w_2\ w_3]$ and $L = S^{-1}\text{diag}(\lambda_1, \lambda_2, \lambda_3)S$, where S is a random 3×3 matrix. We generate random perturbations dV and dW, whose entries obey the standard normal distribution, and we normalize them such that $\|dV\| = \|V\|$ and $\|dW\| = \|W\|$. Then the right and left eigenspace approximations are constructed by the MATLAB command

```
X = V + err*dV;   Y = W + err*dW;
```

such that $\|X - V\|$ is proportional to $\|Y - W\|$. There is no need to normalized X and Y, because the normalization does not change the eigenvalues of the block Rayleigh functional, as is shown in (A.2). The block Rayleigh functional Q is computed by Newton's method with initial iterate L.

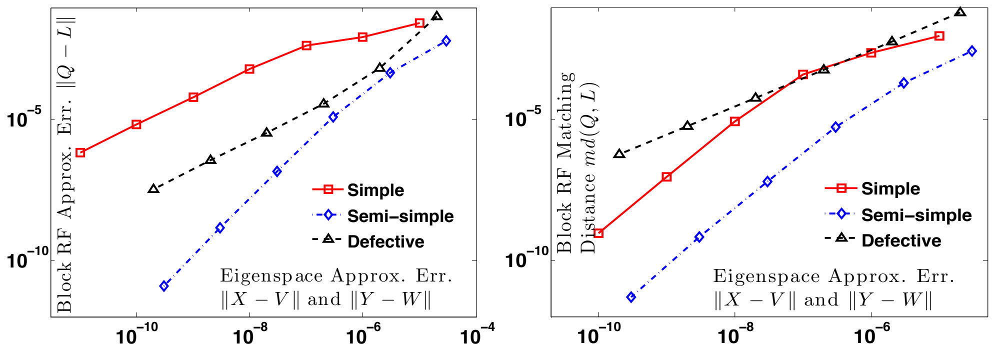

FIG. 6.2. *Two-sided Block Rayleigh functional approximations Left: eigenspace approximation errors* $\|X-V\|$ *and* $\|Y-W\|$ (x-axis) *vs. block Rayleigh functional approximation errors* $\|Q-L\|$ (y-axis) *Right: eigenspace approximation errors* $\|X-V\|$ *and* $\|Y-W\|$ (x-axis) *vs. optimal matching distance* $md(Q,L)$ (y-axis)

The left part of Figure 6.2 shows that Q is an approximation to L of first order accuracy, that is, $\|Q-L\| = \mathcal{O}(\|X-V\|) = \mathcal{O}(\|Y-W\|)$; see the solid line with $\square$ marker. In the right part of Figure 6.2, we plotted the *optimal matching distance* [28, Chapter 4.1] between Q and L against $\|X-V\|$. This distance is defined as

$$md(Q,L) = \min_{\pi(i)} \max_{1\le i\le 3} |\lambda_{\pi(i)}(Q) - \lambda_i(L)|,$$

where π is taken over all permutations of $\{1,2,3\}$; it is a reliable estimate of the approximation of the spectrum of Q to that of L. We see that the eigenvalue approximations are of second order accuracy, i.e., $md(Q,L) = \mathcal{O}(\|X-V\|\|Y-W\|)$.

We repeated the experiments for semi-simple and defective eigenvalues. Note that for the semi-simple eigenvalue, both $\|Q-L\|$ and $md(Q,L)$ are proportional to $\mathcal{O}(\|X-V\|\|Y-W\|)$; see the dash-dot lines with $\Diamond$ markers. The accuracy of Q as an approximation of L is higher than that presented in Theorem 4.10. We have no proof of this observation, but we believe this is due to the fact that $L = S^{-1}\mathrm{diag}(\lambda_1,\lambda_2,\lambda_3)S = \lambda_i I_3$ is a diagonal matrix. For the defective eigenvalue, what we observed for simple eigenvalues holds verbatim; that is, $\|Q-L\|$ and $md(Q,L)$ are proportional to $\mathcal{O}(\|X-V\|)$ and $\mathcal{O}(\|X-V\|\|Y-W\|)$, respectively. Note that in the defective case, the highest accuracy of $\|Q-L\|$ and $md(Q,L)$ is roughly on the order of the square root of machine precision. As we remarked in Section 6.2, this is due to the serious ill-conditioning of the defective eigenpair (λ_4, v_4); see [18].

7. Conclusion. We investigated a few important properties of invariant pairs of nonlinear algebraic eigenvalue problems. We showed that the algebraic, partial, and geometric multiplicities of an eigenvalue of a simple invariant pair are identical to those of this eigenvalue of the nonlinear eigenvalue problem. We then studied the approximation errors and perturbations of simple invariant pairs, and the accuracy of eigenvalue approximations achieved by the block Rayleigh functional. We analyzed the structure of the inverse Fréchet derivative arising in the block version of Newton's method, and we discussed the norm estimate of the inverse derivative that describes the conditioning and sensitivity of simple invariant pairs. Numerical examples are given to illustrate the analysis.

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Appendix A: Proof of Theorem 4.11. The proof consists of three steps. In the first step, we consider a special case where the exact minimal pair $(V, L) \in \mathbb{C}^{n\times k} \times \mathbb{C}^{k\times k}$ is such that L is diagonal and has only one distinct eigenvalue λ; that is, λ is a semi-simple eigenvalue of L of multiplicity k, and it is also a semi-simple eigenvalue of $T(\cdot)$ of multiplicity $g \geq k$. In the second step, we consider a more general case where L is diagonal and has at least two distinct eigenvalues. Finally, we show that the result developed in the first two steps can be extended to a minimal invariant pair (V, L) with non-diagonal L.

We begin with the first step. Let λ be a semi-simple eigenvalue of $T(\cdot)$ whose multiplicity is $g \geq k$, and $\{\varphi_1, \varphi_2, \ldots, \varphi_g\}$ and $\{\psi_1, \psi_2, \ldots, \psi_g\}$ are the corresponding right and left eigenvectors that span $\ker T(\lambda)$ and $\ker\,(T(\lambda))^H$, respectively, such that $\psi_i T'(\lambda)\varphi_j = \delta_{ij}$. Without loss of generality, let $V = [\varphi_1 \varphi_2 \ldots \varphi_k]$, $W = [\psi_1 \psi_2 \ldots \psi_k]$, and $L = \lambda I_k$. Let (X, G) be an approximation to (V, L), and Y an approximation to W. Assume that X is sufficiently close to V in norm, and that the conditions of Theorem 4.10 are satisfied. It then follows that there exists a unique block Rayleigh functional Q such that $Y^H\mathbb{T}(X, Q) = 0$, and $\|Q - L\| \leq \frac{2\delta}{1+\sqrt{1-h}} \leq 2\delta$. Assume that Q is diagonalizable, such that $Q = S_Q\Lambda_Q S_Q^{-1}$ where $\Lambda_Q = \mathrm{diag}(\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_k)$. We know from Gerschgorin theory that for all $i = 1, 2, \ldots, k$,

$$|\tilde{\lambda}_i - \lambda| \leq |Q_{ii} - \lambda| + \sum_{1\leq j\leq k,\, j\neq i} |Q_{ij}| \leq \|Q - L\|_\infty \leq \sqrt{k}\|Q - L\|_F \leq 2\sqrt{k}\delta$$

This means that for each eigenvalue λ of L, there exits a unique eigenvalue $\tilde{\lambda}_i$ of Q such that $|\mu - \lambda| \leq \mathcal{O}(\delta)$. In fact, there are more accurate eigenvalue approximations as we show in the following derivation. Note that since $Y^H\mathbb{T}(X, Q) = 0$, we have

$$Y^H\mathbb{T}(X, Q) = \sum_{i=1}^{m} Y^H A_i X f_i(Q) = \sum_{i=1}^{m} Y^H A_i X S_Q f_i(\Lambda_Q) S_Q^{-1}$$
$$= \sum_{i=1}^{m} Y^H A_i \left(V S_Q + (X - V)S_Q\right) \mathrm{diag}(f_i(\tilde{\lambda}_1), f_i(\tilde{\lambda_2}), \ldots, f_i(\tilde{\lambda_k}))S_Q^{-1} = 0,$$

from which it follows that

$$\text{(A.1)} \qquad \sum_{i=1}^{m} y_j^H A_i \left(V S_Q e_j + (X - V)S_Q e_j\right) f_i(\tilde{\lambda}_j)$$
$$= y_j^H T(\tilde{\lambda}_i) \left(V S_Q e_j + (X - V)S_Q e_j\right) = 0.$$

Obviously, if $\|X - V\|$ is sufficiently small, then the right eigenvector approximation $V S_Q e_j + (X - V)S_Q e_j$ is sufficiently close to the exact right eigenvector $V S_Q e_j$. Assume that the (j, j) entry of S_Q is nonzero, so that $V S_Q e_j$ has a nonzero component of v_j and thus $w_j^H T'(\lambda) V S_Q e_j \neq 0$. It follows that the result shown on the second order accuracy in eigenvalue approximation of the scalar Rayleigh functional can be directly applied to (A.1), such that $|\tilde{\lambda}_j - \lambda| \leq \mathcal{O}(\sin\alpha \sin\beta)$, where $\alpha = \angle(w_j, y_j)$ and $\beta = \angle(V S_Q e_j, V S_Q e_j + (X - V)S_Q e_j)$. This completes the first step of our proof.

To begin the second step, we need to review an important perturbation theorem for block matrices.

PROPOSITION A.1. [27, Chapter 4, Theorem 2.10] *Let* $\|\cdot\|$ *be a consistent matrix norm. Let* $B = \begin{bmatrix} N & H \\ K & M \end{bmatrix}$, *and define* $\mathrm{sep}(N, M) = \inf_{\|P\|=1} \|PN - MP\|$. *If*

$4\|K\|\|H\| \leq \text{sep}^2(N,M)$*, then there exists a unique matrix* P *satisfying* $PN - MP = K - PHP$ *and* $\|P\| \leq 2\frac{\|K\|}{\text{sep}(N,M)}$ *such that*

$$\tilde{B} = \begin{bmatrix} I & 0 \\ -P & I \end{bmatrix} B \begin{bmatrix} I & 0 \\ P & I \end{bmatrix} = \begin{bmatrix} N+HP & H \\ 0 & M-PH \end{bmatrix},$$

where $N+HP$ *and* $M-PH$ *have disjoint spectra.*

Let $\lambda_1,\ldots,\lambda_\ell,\lambda_{\ell+1},\ldots,\lambda_k$ be non-defective eigenvalues of $T(\cdot)$, where $\lambda_1 = \lambda_2 = \ldots = \lambda_\ell$, and they are not equal to any value in the set $\{\lambda_{\ell+1},\ldots,\lambda_k\}$. Let $\{v_i\}$ and $\{w_i\}$ be corresponding right and left eigenvectors, respectively, such that $w_i^H T'(\lambda_1)v_j = \delta_{ij}$ for $1 \leq i,j \leq \ell$ and $w_i^H T'(\lambda_i)v_i = 1$ for $\ell+1 \leq i \leq k$. Let $L = diag(\lambda_1,\ldots,\lambda_\ell,\lambda_{\ell+1},\ldots,\lambda_k)$, $V = [V_1\ V_2] = [\varphi_1 \cdots \varphi_\ell\ \varphi_{\ell+1} \cdots \varphi_k]$, and $W = [W_1\ W_2] = [\psi_1 \cdots \psi_\ell\ \psi_{\ell+1} \cdots \psi_k]$. Let (X,G) be an approximation to (V,L), and Y an approximation to W, such that $\|X-V\|$ and $\|Y-W\|$ are sufficiently small. Assume that the conditions in Theorem 4.10 are satisfied, so that there exists a unique block Rayleigh functional Q such that $Y^T\mathbb{T}(X,G) = 0$, and $\|Q-L\| \leq \frac{2\delta}{1+\sqrt{1-h}} \leq 2\delta$. We see that

$$Q = L + E_Q = \begin{bmatrix} L_1 + E_Q^{11} & E_Q^{12} \\ E_Q^{21} & L_2 + E_Q^{22} \end{bmatrix}, \text{ where}$$
$$L_1 = diag(\lambda_1,\ldots,\lambda_\ell), \quad L_2 = diag(\lambda_{\ell+1},\ldots,\lambda_k), \text{ and}$$
$$\|E_Q^{ij}\| \leq 2\delta\ (i,j = 1,2).$$

Here, note that L_1 and L_2 have disjoint spectra. Since $\|X-V\|$ is sufficiently small, so are δ (see Theorem 4.10) and $\|E_Q^{ij}\|$. Therefore the $(1,1)$ and $(2,2)$ blocks of Q, namely, $L_1 + E_Q^{11}$ and $L_2 + E_Q^{22}$, also have disjoint spectra. By Proposition A.1, there is a unique matrix $P \in \mathbb{C}^{(k-\ell)\times\ell}$ satisfying $\|P\| \leq \frac{2\|E_Q^{21}\|}{\text{sep}(L_1+E_Q^{11},L_2+E_Q^{22})}$ such that

$$\tilde{Q} = \begin{bmatrix} I & 0 \\ -P & I \end{bmatrix} Q \begin{bmatrix} I & 0 \\ P & I \end{bmatrix} = \begin{bmatrix} L_1 + E_Q^{11} + E_Q^{12}P & E_Q^{12} \\ 0 & L_2 + E_Q^{22} - PE_Q^{12} \end{bmatrix},$$

and the spectra of $L_1+E_Q^{11}+E_Q^{12}P$ and $L_2+E_Q^{22}-PE_Q^{12}$ are disjoint. Let $Z \in \mathbb{C}^{\ell\times(k-\ell)}$ be the unique solution of the Sylvester equation

$$Z\left(L_2 + E_Q^{22} - PE_Q^{12}\right) - \left(L_1 + E_Q^{11} + E_Q^{12}P\right)Z = 0\ .$$

Then the block upper-triangular $\tilde{Q}$ can be written as

$$\tilde{Q} = \begin{bmatrix} I & Z \\ 0 & I \end{bmatrix} \begin{bmatrix} L_1 + E_Q^{11} + E_Q^{12}P & 0 \\ 0 & L_2 + E_Q^{22} - PE_Q^{12} \end{bmatrix} \begin{bmatrix} I & -Z \\ 0 & I \end{bmatrix},$$

such that the $(1,1)$ block of the matrix function $f(\tilde{Q})$ is $f(L_1 + E_Q^{11} + E_Q^{12}P)$.

With the above derivation, we can complete the second step of the proof as follows. Let $X = [X_1\ X_2]$ and $Y = [Y_1\ Y_2]$ where $X_1, Y_1 \in \mathbb{C}^{n\times\ell}$ and $X_2, Y_2 \in \mathbb{C}^{n\times(k-\ell)}$. Since the block Rayleigh functional Q satisfies $Y^T\mathbb{T}(X,Q) = 0$, we have

$$\begin{aligned} Y^H\mathbb{T}(X,Q) &= \sum_{j=1}^m Y^H A_j X f_j(Q) = \sum_{j=1}^m Y^H A_j X f_j\left(\begin{bmatrix} I & 0 \\ P & I \end{bmatrix} \tilde{Q} \begin{bmatrix} I & 0 \\ -P & I \end{bmatrix}\right) \\ &= \sum_{j=1}^m [Y_1\ Y_2]^H A_j [X_1\ X_2] \begin{bmatrix} I & 0 \\ P & I \end{bmatrix} f_j(\tilde{Q}) \begin{bmatrix} I & 0 \\ -P & I \end{bmatrix} = 0. \end{aligned}$$

The $(1,1)$ block of the above matrix equation is

$$\sum_{j=1}^{m} Y_1^H A_j (X_1 + X_2 P) f_j (L_1 + E_Q^{11} + E_Q^{12} P) = 0.$$

Here, note that $L_1 + E_Q^{11} + E_Q^{12}P$ is a good approximation to $L_1 = diag(\lambda_1, \ldots, \lambda_\ell)$ since $\|E_Q^{11}\|, \|E_Q^{12}\| \le \mathcal{O}(\delta)$ and $\|P\| \le \mathcal{O}(\|E_Q^{21}\|) \le \mathcal{O}(\delta)$, Y_1 is a good approximation to the left eigenvectors $W_1 = [\psi_1, \ldots, \psi_\ell]$, X_1 is a good approximation to the right eigenvectors $V_1 = [\varphi_1, \ldots, \varphi_\ell]$, and so is $X_1 + X_2 P$. Therefore, the result we developed in the first step can be applied, indicating that the eigenvalues of $L_1 + E_Q^{11} + E_Q^{12}P$ are approximations to λ_1 of second order accuracy. Note that the spectra of $L_1 + E_Q^{11} + E_Q^{12}P$ is a subset of the spectra of $\tilde{Q}$, which is equivalent to that of Q. This completes the second step of the proof.

Finally, for any minimal invariant pair (V', L') involving non-defective eigenvalues of $T(\cdot)$ where L' is a non-diagonal matrix, we can first transform (V', L') to (V, L) with diagonal L and apply the same transformation to the approximate pair (X, G). Specifically, let $L' = S_L L S_L^{-1}$, $V' = V S_L^{-1}$, and consider the transformed approximate pair $(XS_L, S_L^{-1} G S_L)$. If $\|X - V'\|$ is sufficiently small, then

$$\|XS_L - V\| \le \|X - V'\| \|S_L\|$$

is also small as long as $\|S_L\|$ is not too large. Then the above two steps of proof can be applied to the transformed pairs. Note that if the conditions of Theorem 4.10 are satisfied such that there exists a unique block Rayleigh functional in our setting, then the two block Rayleigh functionals Q_a satisfying $Y^H \mathbb{T}(X, Q_a) = 0$ and Q_b satisfying $(YF_1)^H \mathbb{T}(XF_2, Q_b) = 0$ (F_1 and F_2 are any nonsingular $k \times k$ matrices) have identical spectra, because

$$\text{(A.2)} \qquad (YF_1)^H \mathbb{T}(XF_2, Q_b) = \sum_{j=1}^{m} F_1^H Y^H A_j X F_2 f_j(Q_b)$$
$$= \sum_{j=1}^{m} F_1^H Y^H A_j X f_j(F_2 Q_b F_2^{-1}) F_2 = 0 \quad \Longleftrightarrow \quad Y^H \mathbb{T}(X, F_2 Q_b F_2^{-1}) = 0,$$

from which $Q_a = F_2 Q_b F_2^{-1}$ follows. Therefore, the second order accuracy in eigenvalue approximation of the two-sided block Rayleigh functional holds for a pair (X, G) that is sufficiently close to any given minimal invariant pair (V, L) involving only non-defective eigenvalues of $T(\cdot)$.

The above analysis of the two-sided block Rayleigh functional for approximating non-defective eigenvalues can be applied verbatim to the defective eigenvalues. Since the two-sided scalar Rayleigh functional can only achieve the first order accuracy in approximating defective eigenvalues, the same conclusion holds for the two-sided block Rayleigh functionals. This completes the proof.

Appendix B: Proof of Theorem 5.1. The derivation of the norm estimate of $\mathbb{L}_{(V,L)}^{-1}$ consists of two steps. In step 1, we study the structure of $\begin{bmatrix} H & M \\ N & K \end{bmatrix}$, i.e., the matrix representation of $\mathbb{L}_{(V,L)}$. We note that the $(1,1)$ block matrix H is in fact the matrix representation of the functional $\Delta X \to \mathbb{T}(\Delta X, L)$ (this functional is a block generalization of the matrix $T(\lambda_0)$). We have $1 \le \dim(\ker(H)) \le k^2$, and

$\dim(\ker(H)) = k^2$ if and only if L has a unique eigenvalue that is semi-simple. In step 2, using the singular value decomposition of H, we give a 3×3 block matrix representation of $\mathbb{L}_{(V,L)}$ together with its inverse.

We begin with step 1 to study the structure of the matrix representation of $\mathbb{L}_{(V,L)}$ and the dimension of $\ker(H)$. Suppose that L has s distinct eigenvalues $\lambda_1, \ldots, \lambda_s$ with algebraic multiplicities $\{alg_L(\lambda_i)\}$ $(1 \le i \le s)$. It is easy to see that any 2×2 block matrix of the form $\begin{bmatrix} L & \Delta G \\ 0 & L \end{bmatrix}$ with arbitrary $\Delta G \in \mathbb{C}^{k\times k}$ has s distinct eigenvalues $\lambda_1, \ldots, \lambda_s$ with algebraic multiplicities $\{2\,alg_L(\lambda_i)\}$. Note that the size of the largest Jordan block of this block matrix corresponding to λ_i is $2\,alg_L(\lambda_i) \times 2\,alg_L(\lambda_i)$ at most. By the Hermite interpolation theory (see, e.g., [4, Section 4.3.1]), there are polynomials p_j $(1 \le j \le m)$ of degree $d = 2\sum_{i=1}^{s} alg_L(\lambda_i) - 1 = 2k-1$ such that

$$p_j^{(d_i)}(\lambda_i) = f_j^{(d_i)}(\lambda_i),$$

where $1 \le i \le s$, $0 \le d_i \le 2\,alg_L(\lambda_i) - 1$ for each f_j in (2.1). It then follows from the proof of [12, Theorem 10] that $p_j(L) = f_j(L)$ and $\mathbb{D}p_{j(L)}(\Delta G) = \mathbb{D}f_{j(L)}(\Delta G)$ for any ΔG, and therefore f_j can be equivalently replaced with p_j for the Fréchet derivative $\mathbb{L}_{(V,L)}$. Let $p_j(t) = \sum_{r=0}^{d} c_{jr}t^r$, and note that the Fréchet derivative of L^r for $r \ge 1$ is $[\mathbb{D}L^r](\Delta G) = \sum_{i=0}^{r-1} L^i \Delta G L^{r-i-1}$.

We transform $\mathbb{L}_{(V,L)}^{-1}$ into a matrix form to analyze its norm. For this purpose, we define the vectorization of an ordered pair (X, G) as $vec\left((X,G)\right) \equiv \begin{bmatrix} vec(X) \\ vec(G) \end{bmatrix}$. Then, noting that $vec(AXB) = (B^T \otimes A)vec(X)$, we have

$$\text{(B.1)}\ vec\left(\mathbb{L}_{(V,L)}(\Delta X, \Delta G)\right) = \begin{bmatrix} vec\left(\sum_{j=1}^{m} A_j \Delta X p_j(L) + \sum_{j=1}^{m} A_j V \mathbb{D}p_{j(L)}(\Delta G)\right) \\ vec\left(\sum_{j=0}^{\ell-1} W_j^H \Delta X L^j + \sum_{j=1}^{\ell-1} W_j^H V [\mathbb{D}L^j](\Delta G)\right) \end{bmatrix}$$

$$= \begin{bmatrix} vec\left(\sum_{j=1}^{m} A_j \Delta X p_j(L)\right) + vec\left(\sum_{j=1}^{m} A_j V \sum_{r=1}^{d} c_{jr} \sum_{i=0}^{r-1} L^i \Delta G L^{r-i-1}\right) \\ vec\left(\sum_{j=0}^{\ell-1} W_j^H \Delta X L^j\right) + vec\left(\sum_{j=1}^{\ell-1} W_j^H V \sum_{i=0}^{j-1} L^i \Delta G L^{j-i-1}\right) \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{j=1}^{m} p_j(L)^T \otimes A_j & \sum_{j=1}^{m}\sum_{r=1}^{d}\sum_{i=0}^{r-1} (L^{r-i-1})^T \otimes (c_{jr} A_j V L^i) \\ \sum_{j=0}^{\ell-1} (L^j)^T \otimes W_j^H & \sum_{j=1}^{\ell-1}\sum_{i=0}^{j-1} (L^{j-i-1})^T \otimes (W_j^H V L^i) \end{bmatrix} \begin{bmatrix} vec(\Delta X) \\ vec(\Delta G) \end{bmatrix}$$

$$\equiv \begin{bmatrix} H_{nk\times nk} & M_{nk\times k^2} \\ N_{k^2\times nk} & K_{k^2\times k^2} \end{bmatrix} \begin{bmatrix} vec(\Delta X) \\ vec(\Delta G) \end{bmatrix}.$$

To reveal the structure of the 2×2 block matrix just defined, we need to study the above $(1,1)$ block H and $\dim(\ker(H))$. Let $J_L = Z^{-1}LZ$ be the Jordan canonical form of L. First, suppose that J_L has only one distinct eigenvalue λ_0 such that $J_L = \operatorname{diag}\left(J_{k_1}(\lambda_0), J_{k_2}(\lambda_0), \ldots, J_{k_g}(\lambda_0)\right)$ with $k_1 \ge k_2 \ge \ldots \ge k_g$, where J_{k_i} is a Jordan block of size $k_i \times k_i$. Then we have

$$H = \sum_{j=1}^{m} p_j(L)^T \otimes A_j = \sum_{j=1}^{m} \left(Z p_j(J_L) Z^{-1}\right)^T \otimes A_j$$
$$= \sum_{j=1}^{m} \left(Z^{-T} p_j(J_L)^T Z^T\right) \otimes A_j = (Z^{-T} \otimes I_n)\left(\sum_{j=1}^{m} p_j(J_L)^T \otimes A_j\right)(Z^T \otimes I_n).$$

Let $\widehat{H} = \sum_{j=1}^{m} p_j(J_L)^T \otimes A_j$. Since $Z^{-T} \otimes I_n$ and $Z^T \otimes I_n$ are nonsingular, we have $\dim(\ker(H)) = \dim(\ker(\widehat{H}))$.

Now consider the top left $nk_1 \times nk_1$ submatrix of $\widehat{H}$

$$\begin{aligned}
\widehat{H}_1 &= \textstyle\sum_{j=1}^{m} p_j(J_{k_1}(\lambda_0))^T \otimes A_j \\
&= \sum_{j=1}^{m} \begin{bmatrix} p_j(\lambda_0)A_j & & & & \\ p_j'(\lambda_0)A_j & p_j(\lambda_0)A_j & & & \\ \frac{p_j''(\lambda_0)}{2}A_j & p_j'(\lambda_0)A_j & p_j(\lambda_0)A_j & & \\ \vdots & \vdots & \vdots & \ddots & \\ \frac{p_j^{(k_1-1)}(\lambda_0)}{(k_1-1)!}A_j & \cdots & \cdots & p_j'(\lambda_0)A_j & p_j(\lambda_0)A_j \end{bmatrix} \\
&= \begin{bmatrix} T(\lambda_0) & & & & \\ T'(\lambda_0) & T(\lambda_0) & & & \\ \frac{T''(\lambda_0)}{2} & T'(\lambda_0) & T(\lambda_0) & & \\ \vdots & \vdots & \vdots & \ddots & \\ \frac{T^{(k_1-1)}(\lambda_0)}{(k_1-1)!} & \cdots & \cdots & T'(\lambda_0) & T(\lambda_0) \end{bmatrix}.
\end{aligned}$$

Recall from Section 3 that for a simple invariant pair (V, L), the Jordan block $J_{k_1}(\lambda_0)$ of L corresponds to a Jordan chain $\{\varphi_{1,0}, \varphi_{1,1}, \ldots, \varphi_{1,k_1-1}\}$ associated with λ_0 of the nonlinear eigenvalue problem (2.1). By the definition of Jordan chains (2.2), we have that $\varphi_1 \equiv \left[\varphi_{1,0}^T, \varphi_{1,1}^T, \ldots, \varphi_{1,k_1-1}^T\right]^T \in \ker(\widehat{H}_1)$.

Consider the second Jordan block $J_{k_2}(\lambda_0)$ and the corresponding matrix $\widehat{H}_2 = \sum_{j=1}^{m} p_j(J_{k_2}(\lambda_0))^T \otimes A_j$, the second block diagonal submatrix of $\widehat{H}$. Let the associated Jordan chain be $\{\varphi_{2,0}, \ldots, \varphi_{2,k_2-1}\}$. Then $\varphi_2 \equiv \left[\varphi_{2,0}^T, \ldots, \varphi_{2,k_2-1}^T\right]^T \in \ker(\widehat{H}_2)$. Here, if $k_2 = k_1$, then $\widehat{H}_1 = \widehat{H}_2$, and $\varphi_1, \varphi_2 \in \ker(\widehat{H}_1) = \ker(\widehat{H}_2)$. That is, Jordan chains of the same length corresponding to λ_0 can be exchanged in this setting to construct the null space vectors. Similarly, suppose that $k_1 = k_2 = \ldots = k_p > k_{p+1} \geq \ldots \geq k_q$, then $\varphi_1, \varphi_2, \ldots, \varphi_p \in \ker(\widehat{H}_i)$ $(1 \leq i \leq p)$, and

$$\text{(B.2)} \quad \begin{bmatrix} \varphi_1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} \varphi_p \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \varphi_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ \varphi_p \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \varphi_1 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \varphi_p \end{bmatrix}$$
$$\in \ker\left(\operatorname{diag}(\widehat{H}_1, \widehat{H}_2, \cdots, \widehat{H}_p)\right).$$

Note that the leading vectors in the p Jordan chains, namely, $\{\varphi_{1,0}, \varphi_{2,0}, \ldots, \varphi_{p,0}\}$ are linearly independent (see Theorem 3.1). Therefore $\{\varphi_1, \varphi_2, \ldots, \varphi_p\}$ are linearly independent, and so are the p^2 vectors in (B.2).

Therefore, if the g Jordan blocks can be grouped into s collections such that each collection contains p_i $(1 \leq i \leq s)$ Jordan blocks of the same size, and the Jordan blocks in two collections are of different size, then we have $\dim(\ker(\widehat{H})) = \sum_{i=1}^{s} p_i^2$. If L has two or more distinct eigenvalues, the same calculation can be applied to each distinct eigenvalue, and we can see easily that $\dim(\ker(H)) = \dim(\ker(\widehat{H}))$ is the sum of the dimensions of the null spaces for each distinct eigenvalue.

For example, suppose that L has 2 distinct eigenvalues λ_0 and λ_1. Assume that for λ_0, there are 3 Jordan blocks of size 4×4, 1 Jordan block of size 3×3, and 2

Jordan blocks of size 1×1; for λ_1, there are 1 Jordan block of size 2×2 and 4 Jordan blocks of size 1×1. Then $\dim(\ker(H)) = (3^2+1^2+2^2)+(1^2+4^2) = 31$. In particular, consider the following three scenarios:

1. L has only one distinct eigenvalue, and there is only 1 Jordan block of size $k\times k$. Then $\dim(\ker(H)) = 1$, the minimum value;
2. L has k distinct simple eigenvalues. Then $\dim(\ker(H)) = k$;
3. L has only one distinct eigenvalue and the eigenvalue is semi-simple (k Jordan blocks of size 1×1). Then $\dim(\ker(H)) = k^2$.

From the above discussion, it is not hard to see that k^2 is the maximum value of $\dim(\ker(H))$, and it can be achieved if and only if $\Lambda(L) = \{\lambda_0\}$ and λ_0 is semi-simple. This concludes step 1.

In step 2, we give a 3×3 block matrix representation of $\mathbb{L}^{-1}_{(V,L)}$. Assume that $\dim(\ker(H)) = r$ with $1\le r\le k^2$, and the singular value decomposition of H is $H = Y_a \begin{bmatrix} \Sigma_{11} & 0 \\ 0 & 0 \end{bmatrix} Y_b^H$, where $\Sigma_{11}\in\mathbb{C}^{(nk-r)\times(nk-r)}$ has all the nonzero singular values of H on its diagonal, say, in decreasing magnitude. Define

$$\text{(B.3)}\quad F_* \equiv \begin{bmatrix} Y_a^H & 0 \\ 0 & I_{k^2} \end{bmatrix}\begin{bmatrix} H & M \\ N & K \end{bmatrix}\begin{bmatrix} Y_b & 0 \\ 0 & I_{k^2} \end{bmatrix} = \begin{bmatrix} Y_a^H H Y_b & Y_a^H M \\ N Y_b & K \end{bmatrix} = \begin{bmatrix} \Sigma_{11} & 0 & M_{13} \\ 0 & 0 & M_{23} \\ N_{31}^H & N_{32}^H & K \end{bmatrix},$$

where $M_{13}\in\mathbb{C}^{(nk-r)\times k^2}$, $M_{23}\in\mathbb{C}^{r\times k^2}$, $N_{31}^H\in\mathbb{C}^{k^2\times(nk-r)}$, $N_{32}^H\in\mathbb{C}^{k^2\times r}$, $Y_a^H M = \begin{bmatrix} M_{13} \\ M_{23} \end{bmatrix}$ and $NY_b = \begin{bmatrix} N_{31}^H & N_{32}^H \end{bmatrix}$. If F_* is nonsingular, then $\|F_*^{-1}\| = \left\| \begin{bmatrix} H & M \\ N & K \end{bmatrix}^{-1} \right\|$ in any unitary invariant norm.

For a simple invariant pair (V,L), Theorem 2.4 shows that the Fréchet derivative $\mathbb{L}_{(V,L)}$ is invertible, and therefore, its matrix representation $\begin{bmatrix} H & M \\ N & K \end{bmatrix}$ is nonsingular. It follows that F_* is nonsingular, and so is the Schur complement of Σ_{11}, namely,

$$\begin{bmatrix} 0 & M_{23} \\ N_{32}^H & K \end{bmatrix} - \begin{bmatrix} 0 \\ N_{31}^H \end{bmatrix} \Sigma_{11}^{-1} \begin{bmatrix} 0 & M_{13} \end{bmatrix} = \begin{bmatrix} 0 & M_{23} \\ N_{32}^H & K - N_{31}^H \Sigma_{11}^{-1} M_{13} \end{bmatrix}.$$

As a result, N_{32}^H and M_{23} must be of full rank. In the special case where L has exactly one distinct eigenvalue that is semi-simple, then $r = k^2$, and F_* is nonsingular if and only if the square matrices N_{32}^H and M_{23} are nonsingular.

If F_* is nonsingular, we can obtain F_*^{-1} by block elimination as follows:

$$\begin{bmatrix} \Sigma_{11}^{-1} - \Sigma_{11}^{-1} M_{13} Q_3^{-1} Q_0 & \Sigma_{11}^{-1} M_{13} Q_3^{-1} N_{32}^H & -\Sigma_{11}^{-1} M_{13} Q_3^{-1}\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) \\ -(N_{32}^H)_L^{-1} N_{31}^H \Sigma_{11}^{-1} - Q_2 Q_3^{-1} Q_0 & I + Q_2 Q_3^{-1} N_{32}^H & (N_{32}^H)_L^{-1} - Q_2 Q_3^{-1}\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) \\ Q_3^{-1} Q_0 & -Q_3^{-1} N_{32}^H & Q_3^{-1}\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) \end{bmatrix},$$

where $(N_{32}^H)_L^{-1} = (N_{32} N_{32}^H)^{-1} N_{32} \in \mathbb{C}^{r\times k^2}$ is the left inverse of N_{32}^H, and

$$\begin{aligned} Q_0 &= -\left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) N_{31}^H \Sigma_{11}^{-1} \in \mathbb{C}^{k^2\times(nk-r)}, \\ Q_1 &= K_{33} - N_{31}^H \Sigma_{11}^{-1} M_{13} \in \mathbb{C}^{k^2\times k^2}, \\ Q_2 &= M_{23} + (N_{32}^H)_L^{-1} Q_1 \in \mathbb{C}^{r\times k^2}, \\ Q_3 &= Q_1 - N_{32}^H Q_2 = \left(I - N_{32}^H (N_{32}^H)_L^{-1}\right) Q_1 - N_{32}^H M_{23} \in \mathbb{C}^{k^2\times k^2}. \end{aligned}$$

This completes step 2, where we obtained a block matrix form of $\mathbb{L}^{-1}_{(V,L)}$. Theorem 5.1 is thus established.

Remark B.1. For linear eigenproblems, let (V, L) be an exact minimal invariant pair of $T(\lambda) = \lambda I - A$. Then the functional $\Delta X \to \mathbb{T}(\Delta X, L)$, which has the matrix representation H as discussed in Theorem 5.1, has the null space

$$\ker(\mathbb{T}(\cdot, L)) = \{X = VK \,:\, K \in \mathbb{C}^{k\times k} \text{ which solves } LK - KL = 0\}.$$

The dimension of this null space equals the dimension of the null space of the linear map $K \to LK - KL$, and this dimension can be explicitly dertermined from the Jordan canonical form of L; see [5] for details.

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