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LOCAL CONVERGENCE OF NEWTON-LIKE METHODS FOR DEGENERATE EIGENVALUES OF NONLINEAR EIGENPROBLEMS*

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Abstract. We study the local convergence rates of several single-vector Newton-like methods for the solution of a semi-simple or defective eigenvalue of nonlinear algebraic eigenvalue problems of the form $T(\lambda)v = 0$. This problem has not been fully understood, since the Jacobian associated with the single-vector Newton's method is singular at the desired eigenpair, and the standard convergence theory is not applicable. In addition, Newton's method generally converges only linearly towards singular roots. In this paper, we show that faster convergence can be achieved for degenerate eigenvalues. For semi-simple eigenvalues, we show that the convergence of Newton's method, Rayleigh functional iteration and the Jacobi-Davidson method are quadratic, and the latter two converge cubically for locally symmetric problems. For defective eigenvalues, all these methods converge only linearly in general. We then study two accelerated methods for defective eigenvalues, which exhibit quadratic convergence and require the solution of two linear systems per iteration. The results are illustrated by numerical experiments.

Key words. nonlinear eigenvalue problems, degenerate eigenvalues, Jordan chains, Newton's method, inverse iteration, Rayleigh functionals, Jacobi-Davidson method

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

1. Introduction.

In this paper, we study the local convergence rates of several single-vector Newton-like methods for the solution of a degenerate eigenvalue λ and a corresponding eigenvector v of the nonlinear algebraic eigenvalue problem of the form

$$T(\lambda)v = 0, \tag{1.1}$$

where $T(\cdot) : U \to \mathbb{C}^{n\times n}$ is holomorphic on a domain $U \subset \mathbb{C}$, $\lambda \in U$ and $v \in \mathbb{C}^n \setminus \{0\}$. λ is an eigenvalue of $T(\cdot)$ if and only if $T(\lambda)$ is singular. Assume that $\det T(\cdot) \not\equiv 0$ in any neighborhood of λ; that is, eigenvalues of $T(\cdot)$ are isolated. The algebraic multiplicity of an eigenvalue λ of (1.1) is defined as the multiplicity of λ as a root of the characteristic function $\det T(\mu)$. The eigenvalue λ is called *degenerate* if its algebraic multiplicity larger than one. A degenerate eigenvalue λ is called *semi-simple* if its geometric multiplicity, defined as the dimension of $\text{null}\,(T(\lambda))$, equals its algebraic multiplicity; it is called *defective* if its geometric multiplicity is smaller than its algebraic multiplicity.

Our study of numerical methods for degenerate eigenvalues of (1.1) is motivated by recent rapid development of theory and algorithms for nonlinear eigenvalue problems. These problems arise in a variety of applications, such as vibrational analysis of structures, stability analysis of fluid flows, optimal control problems, quantum mechanics, and delay differential equations; see, e.g., [17, 18, 31] and references therein. Polynomial and rational eigenvalue problems, which can be transformed via *linearization* into standard linear eigenvalue problems of dimensions multiple times larger, have been studied intensively due to their wide applications [14, 15, 28]. For these problems of small or medium size, linearization is usually the most effective approach. On the other hand, for very large or irrational (truly nonlinear) problems where linearization is not effective or applicable, or if there are only a small number of eigenpairs of interest, other methods might be more appropriate. For example, one can use the contour

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integral method [1, 5, 9] to find initial approximations to the eigenvalues in a specified domain, and apply Newton-like methods to refine the eigenpair approximations.

Variants of Newton-like methods have been proposed and studied for the solution of a single eigenpair of the nonlinear eigenvalue problem (1.1); see the early works [21, 22, 24], a few recent developments [4, 11, 25, 27], and a study of inexact variants of these algorithms [29]. In all these references, the analyses are developed only for *simple* eigenpairs, and the convergence of Newton-like methods are generally quadratic (possibly cubic for problems with local symmetry). However, degenerate eigenpairs also arise in important scenarios such as certain gyroscopic systems, hyperbolic Hermitian polynomial problems, and some delay differential equations, for which the understanding of fast convergent Newton-like methods is not complete. The major difficulty is that the Jacobian (Fréchet derivative) of the augmented system of problem (1.1) at the desired degenerate eigenpair is singular, and the standard convergence theory of Newton's method is not directly applicable. To work around this difficulty, a block version of Newton's method was proposed to compute a simple invariant pair involving the whole eigenspace of the desired degenerate eigenvalues [13], where in each iteration the number of linear systems to be solved equals at least the sum of algebraic multiplicities of all these eigenvalues. Therefore, this method could be prohibitive for degenerate eigenvalues of high algebraic multiplicities.

For many applications, fortunately, we are mostly interested in eigenvalues and a single eigenvector. In this case, single-vector Newton-like methods are probably the most suitable algorithms. The main purpose of this paper is to gain a better understanding of several fast convergent single-vector Newton-like methods for the solution of a degenerate eigenpair of problem (1.1). We assume that the initial approximation to the desired eigenpair is available, and we investigate the local convergence rates of inverse iteration, Rayleigh functional iteration (RFI), and the single-vector Jacobi-Davidson (JD) method. For semi-simple eigenvalues, we show that the local convergence of these algorithms is quadratic or cubic, respectively, if the local symmetry of $T(\cdot)$ is absent or present; in other words, the local convergence rates of the Newton-like methods for semi-simple eigenpairs are identical to those for simple ones. For defective eigenvalues, on the other hand, we show that the convergence of these methods is in general only linear. We then propose two accelerated variants of Newton's method, which exhibit locally quadratic convergence at the cost of solving two linear systems per iteration.

The utility and limitation of the algorithms for defective eigenpairs discussed in this paper need to be emphasized. In particular, it is well known that the computation of defective eigenpairs (eigenvalues and associated eigenvectors alone, excluding the generalized eigenvectors) is an ill-posed problem. A small perturbation of the matrix pencil of order ϵ generally leads to a scattering of a defective eigenvalue λ by a magnitude of $\epsilon^{1/m}$, where m is the length of the longest Jordan chain; see, e.g., [19, 20] and references therein. Therefore, the computation of defective eigenpairs alone is relevant only for those with short Jordan chains (m small) and where moderate accuracy is sufficient for the applications. On the other hand, simple invariant pairs involving a defective eigenpair together with all associated generalized eigenvectors are much less sensitive to perturbations, and therefore the computation of these pairs could be performed to high accuracy; see, for example, [3, 30]. To this end, one may again refer to the block version of Newton's method [13], which is more expensive than the single-vector methods studied in this paper.

The rest of the paper is organized as follows. In Section 2 we review some defini-

tions and preliminary results for degenerate eigenvalues. In Section 3, we show that the singularity of the Jacobian of the augmented system at the desired semi-simple eigenpair has no impact on the local quadratic convergence of inverse iteration; in addition, RFI and single-vector JD converge quadratically or cubically towards a semi-simple eigenpair, respectively, for locally nonsymmetric or symmetric problems. We then show in Section 4 that the convergence of inverse iteration, RFI and single-vector JD towards a defective eigenpair is in general only linear, and we propose two accelerated algorithms that converge quadratically. Numerical experiments are provided throughout the paper to illustrate the convergence results. Section 5 is the conclusion of the paper.

2. Preliminaries. In this section, we review some preliminary results on degenerate eigenvalues for the study of local convergence of Newton-like methods. Theories for semi-simple and defective eigenvalues can be presented in a uniform way, yet we review them separately for the purpose of clarity. For the two types of degenerate eigenvalues, as we shall see, there exist important differences in the structure of the resolvent $T(\mu)^{-1}$ near the eigenvalue, and the sets of right and left eigenvectors satisfy different normalization conditions. These properties are fundamental in the understanding of the quadratic (possibly cubic) and linear convergence of Newton-like methods, respectively, for a semi-simple and a defective eigenpair.

2.1. Semi-simple eigenvalues. Let λ be an eigenvalue of (1.1), $alg_T(\lambda)$ be the algebraic multiplicity of λ, i.e., the multiplicity of λ as a root of the characteristic function $\det T(\mu)$, and $geo_T(\lambda) = \dim(\operatorname{null} T(\lambda))$ be the geometric multiplicity. It can be shown that $alg_T(\lambda) \geq geo_T(\lambda)$. Then λ is semi-simple if $alg_T(\lambda) = geo_T(\lambda) \geq 2$. Intuitively speaking, a semi-simple eigenpair can be considered as a set of multiple simple eigenpairs sharing an identical eigenvalue. This perspective is helpful for our understanding of the quadratic convergence of Newton-like methods in this case.

The major theorem on the structure of the resolvent $T(\mu)^{-1}$ near a semi-simple eigenvalue and the normalization condition of the sets of left and right eigenvectors is described as follows, and it can be obtained directly from Theorem A.10.2 of [12], where all Jordan chains are of length 1.

THEOREM 2.1. *Let T be a Fredholm holomorphic operator function in a neighborhood of a semi-simple eigenvalue $\lambda \in U$. Let $alg_T(\lambda) = J$, and $\{\varphi_k\}$ $(k = 1, \ldots, J)$ be the corresponding right eigenvectors. Then there exists a unique set of corresponding left eigenvectors $\{\psi_k\}$ $(k = 1, \ldots, J)$ such that in a neighborhood of λ*

$$T(\mu)^{-1} = \sum_{k=1}^{J} \frac{\langle \cdot, \psi_k \rangle \varphi_k}{\mu - \lambda} + Q(\mu),$$

where Q is holomorphic in a neighborhood of λ. The two sets of eigenvectors satisfy the following normalization condition

$$\langle T'(\lambda)\varphi_k, \psi_j \rangle = \delta_{jk}, \quad (j, k = 1, \ldots, J). \tag{2.1}$$

In addition, the right eigenvectors satisfy

$$T(\lambda)Q(\lambda)T'(\lambda)\varphi_k = 0, \quad (k = 1, \ldots, J). \tag{2.2}$$

Note that λ is a simple eigenvalue if $J = 1$. Therefore, we assume throughout the paper that $J \geq 2$ for the semi-simple case.

Let $x \neq 0$ be a right eigenvector approximation which has a significant component in $\text{span}\{\varphi_1, \ldots, \varphi_J\}$. We first give a decomposition of x which we use later for the study of the local convergence of Rayleigh functional iteration. Let $G \in \mathbb{C}^{J\times J}$ be a nonsingular matrix, $\Phi_J = [\varphi_1 \ \ldots \ \varphi_J]G$ and $\Psi_J = [\psi_1 \ \ldots \ \psi_J]G^{-*}$ such that

$$\Psi_J^* T'(\lambda)\Phi_J = I_J. \tag{2.3}$$

From (2.1) we know that both $T'(\lambda)\Phi_J$ and $\Psi_J^* T'(\lambda)$ are of full rank. Let $W_{n-J} \in \mathbb{C}^{n\times(n-J)}$ and $U_{n-J} \in \mathbb{C}^{n\times(n-J)}$, respectively, have orthonormal columns such that

$$W_{n-J}^* T'(\lambda)\Phi_J = 0_{(n-J)\times J} \quad \text{and} \quad \Psi_J^* T'(\lambda) U_{n-J} = 0_{J\times(n-J)}. \tag{2.4}$$

Assume that $x \notin \text{range}(U_{n-J})$, such that $\|\Psi_J^* T'(\lambda)x\| \neq 0$. A decomposition of x can be formed as follows:

$$x = \gamma(cv + sg), \tag{2.5}$$

where

$$\begin{aligned} &\gamma = \left\| \begin{bmatrix} \Psi_J^* \\ W_{n-J}^* \end{bmatrix} T'(\lambda)x \right\|, \quad c = \frac{\|\Psi_J^* T'(\lambda)x\|}{\gamma}, \quad s = \frac{\|W_{n-J}^* T'(\lambda)x\|}{\gamma}, \\ &v = \Phi_J \frac{\Psi_J^* T'(\lambda)x}{\|\Psi_J^* T'(\lambda)x\|}, \quad \text{and} \quad g = \frac{1}{s}\left(\frac{x}{\gamma} - cv\right). \end{aligned} \tag{2.6}$$

Here, γ is a generalized norm of x, and c and s with $c^2 + s^2 = 1$ are generalized sine and cosine, respectively, of the angle between x and $v \in \text{span}\{\varphi_1, \ldots, \varphi_J\}$. It can be shown without difficulty that

$$\Psi_J^* T'(\lambda)g = 0 \quad \text{and} \quad \|W_{n-J}^* T'(\lambda)g\| = 1, \tag{2.7}$$

and thus $g \in \text{range}(U_{n-J})$ is an error vector normalized as above. The eigenvector approximation error can be measured by the generalized sine s or tangent $t = s/c$.

2.2. Defective eigenvalues. An eigenvalue λ of (1.1) is defective if $alg_T(\lambda) > geo_T(\lambda)$. This definition is consistent with that for eigenvalues of a matrix.

For a defective eigenvalue λ, the structure of the resolvent $T(\mu)^{-1}$ near λ and the normalization condition of the sets of left and right eigenvectors are more complicated than they are in the semi-simple case.

DEFINITION 2.2. *Let λ be a defective eigenvalue of the holomorphic operator $T(\cdot)$ and $\varphi_{\cdot,0}$ a corresponding right eigenvector. Then the nonzero vectors $\varphi_{\cdot,1}, \ldots, \varphi_{\cdot,m-1}$ are called generalized eigenvectors if*

$$\sum_{j=0}^{n} \frac{1}{j!} T^{(j)}(\lambda)\varphi_{\cdot,n-j} = 0, \quad n = 1, \ldots, m-1, \tag{2.8}$$

where $T^{(j)}(\lambda) = \frac{d^j}{d\mu^j} T(\mu)|_{\mu=\lambda}$. Then the ordered collection $\{\varphi_{\cdot,0}, \varphi_{\cdot,1}, \ldots, \varphi_{\cdot,m-1}\}$ is called a right Jordan chain corresponding to λ. If (2.8) is satisfied for some $m = m_*$ and no more vectors can be introduced such that (2.8) is satisfied for $m = m_* + 1$, then m_* is called the length of the Jordan chain and a partial multiplicity of λ.

Similarly, let $\psi_{\cdot,0}$ be a left eigenvector of λ. One can define a left Jordan chain $\psi_{\cdot,0}, \psi_{\cdot,1}, \ldots, \psi_{\cdot,m-1}$ by replacing $T^{(j)}\varphi_{\cdot,n-j}$ in (2.8) with $\psi_{\cdot,n-j}^* T^{(j)}$.

The structure of the resolvent $T(\mu)^{-1}$ near a defective λ is described as follows (c.f. Theorem A.10.2 of [12]).

THEOREM 2.3. *Let $T : U \to \mathbb{C}^{n\times n}$ be a Fredholm holomorphic function in a neighborhood of a defective eigenvalue λ of T, and J and $m_1, \ldots, m_J$ be the geometric and partial multiplicities of λ. Suppose that $\{\varphi_{k,s}\}$, $k = 1, \ldots, J$, $s = 0, \ldots, m_k - 1$ is a canonical system of right Jordan chains of T corresponding to λ. Then*
(i) *There is a unique canonical system of left Jordan chains $\{\psi_{k,s}\}$, $k = 1, \ldots, J$, $s = 0, \ldots, m_k - 1$ such that in a neighborhood of λ*

$$T(\mu)^{-1} = \sum_{k=1}^{J} \sum_{h=0}^{m_k-1} \frac{\sum_{s=0}^{h} \langle \cdot, \psi_{k,s}\rangle \varphi_{k,h-s}}{(\mu-\lambda)^{m_k-h}} + Q(\mu), \tag{2.9}$$

where Q is holomorphic in a neighborhood of λ.
(ii) *The left Jordan chains $\{\psi_{k,s}\}$ in* (i) *satisfy the following normalization conditions*

$$\begin{aligned} \sum_{s=0}^{\ell} \sum_{\sigma=s+1}^{m_k+s} \frac{1}{\sigma!} \langle T^{(\sigma)}(\lambda)\varphi_{k,m_k+s-\sigma}, \psi_{j,\ell-s}\rangle &= \delta_k^j \delta_\ell^0, \\ \sum_{s=0}^{\ell} \sum_{\sigma=s+1}^{m_k+s} \frac{1}{\sigma!} \langle T^{(\sigma)}(\lambda)\varphi_{k,\ell-s}, \psi_{j,m_k+s-\sigma}\rangle &= \delta_k^j \delta_\ell^0, \end{aligned} \tag{2.10}$$

where $\psi_{j,p} = 0$, $\varphi_{k,q} = 0$ for $p \geq m_j, q \geq m_k$.

An important observation of the sets of right and left eigenvectors associated with a defective eigenvalue can be derived from Theorem 2.3. Note from Definition 2.2 of Jordan chains that $T(\lambda)\varphi_{k,1} + T'(\lambda)\varphi_{k,0} = 0$. Premultiplying by $\psi_{j,0}^*$, we have

$$\psi_{j,0}^* T(\lambda)\varphi_{k,1} + \psi_{j,0}^* T'(\lambda)\varphi_{k,0} = \psi_{j,0}^* T'(\lambda)\varphi_{k,0} = 0 \tag{2.11}$$

for any $j, k = 1, \ldots, J$. We shall see later that this property plays a critical role in the linear convergence of Newton-like methods towards defective eigenvalues.

2.3. Review of Newton-like algorithms. Consider the solution of a single eigenpair (λ, v) under a normalization condition of problem (1.1)

$$F(\lambda, v) = \begin{bmatrix} T(\lambda)v \\ u^*v - 1 \end{bmatrix} = 0, \tag{2.12}$$

where $u \in \mathbb{C}^n$ is a fixed normalization vector such that $u \not\perp v$; see, e.g., [18, 24]. This nonlinear system of equations involving $n + 1$ variables is usually referred to as the augmented system of problem (1.1). Application of Newton's method to the augmented system leads to an iteration scheme as follows:

$$\begin{bmatrix} x_{k+1} \\ \mu_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ \mu_k \end{bmatrix} - \begin{bmatrix} T(\mu_k) & T'(\mu_k)x_k \\ u^* & 0 \end{bmatrix}^{-1} \begin{bmatrix} x_k \\ \mu_k \end{bmatrix}, \tag{2.13}$$

where the computation of the new eigenvector iterate x_{k+1} and the new eigenvalue iterate μ_{k+1} are performed simultaneously by solving a linear system involving the Jacobian of order $n + 1$. In general, it is more convenient to solve a linear system involving a coefficient matrix of order n to compute x_{k+1}, and then update μ_{k+1}

correspondingly. To this end, we exploit the structure of the block inverse of the Jacobian and obtain inverse iteration as follows:

$$\left\{\begin{array}{l} p_k = T^{-1}(\mu_k)T'(\mu_k)x_k \\ x_{k+1} = \dfrac{1}{u^*p_k}p_k \\ \mu_{k+1} = \mu_k - \dfrac{1}{u^*p_k} \end{array}\right. , \tag{2.14}$$

which is mathematically equivalent to Newton's method. Inverse iteration is generally used as a substitute of the original Newton's method (2.13), and its convergence analysis is usually carried out using theories of the latter.

Here, we would like to point out that for a degenerate λ with $geo_T(\lambda) = J > 1$, $T(\lambda) = 0$ together with a single normalization vector may not uniquely determine the eigenvector v, since there could be infinitely many ways to form $v \in \text{span}\{\varphi_1, \cdots, \varphi_J\}$ such that $u^*v = 1$ holds. In many cases, fortunately, one is mostly interested in the computation of the eigenvalue alone, and any single eigenvector $v \in \text{span}\{\varphi_1, \cdots, \varphi_J\}$ would satisfy the needs of the applications. We assume this is the case throughout the paper, so that the study of single-vector Newton-like algorithms is most appropriate for this purpose. If the whole eigenspace of a degenerate eigenvalue is needed, one may have to use a block variant of Newton's method based on invariant pairs [13].

inverse iteration can be modified to incorporate potentially more accurate eigenvalue approximation, so that the convergence can be accelerated for *locally symmetric* problems, i.e., those where $T(\lambda)$ is real (skew) symmetric, complex (skew) Hermitian, or complex (skew) symmetric. The most important variant of this type is the Rayleigh functional iteration (RFI), a natural generalization of Rayleigh quotient iteration (RQI) to the nonlinear eigenvalue problems. Given a right eigenvector approximation $x_k \approx v$, one can choose some auxiliary vector y_k, such that $y_k^*T(\rho_k)x_k = 0$ for some scalar ρ_k, and $\rho_k = \rho_F(x_k; T, y_k)$ is called the value of the nonlinear Rayleigh functional $\rho_F(\cdot; T, y)$; see [26] and references therein. The RFI is described as follows:

$$\left\{\begin{array}{l} \text{choose vector } y_k \text{ and compute } \rho_k = \rho_F(x_k; T, y_k) \text{ s.t. } y_k^*T(\rho_k)x_k = 0; \\ p_k = T^{-1}(\rho_k)T'(\rho_k)x_k; \\ \text{normalize } p_k \text{ and assign it to } x_{k+1}. \end{array}\right. \tag{2.15}$$

RFI bears a close connection to the single-vector Jacobi-Davidson (JD) method, another type of most widely used Newton-like eigenvalue algorithms. Starting with an eigenvector approximation x_k and its corresponding Rayleigh functional value ρ_k, single-vector JD solves a correction equation for a correction vector Δx_k such that the new eigenvector approximation is $x_{k+1} = x_k + \Delta x_k$. The correction equation of JD is a projection (restriction) of the linear system arising in RFI onto a $n-1$ dimensional complementary space of $\text{span}\{x_k\}$. One can construct different variants of the JD correction equation. We focus our study on one variant, which assumes a general form and has been used to compute a simple eigenpair in [29]:

$$\left\{\begin{array}{l} \text{choose vector } y_k \text{ and compute } \rho_k = \rho_F(x_k; T, y_k) \\ \quad \text{s.t. } y_k^*T(\rho_k)x_k = 0 \text{ and } y_k^*T'(\rho_k)x_k \neq 0 \\ \text{define } \Pi_k^{(1)} = I - \dfrac{T'(\rho_k)x_k y_k^*}{y_k^*T'(\rho_k)x_k}, \Pi_k^{(2)} = I - \dfrac{x_k u^*}{u^*x_k}, \text{ and solve the correction} \\ \quad \text{equation } \Pi_k^{(1)}T(\rho_k)\Pi_k^{(2)}\Delta x_k = -T(\rho_k)x_k \text{ for } \Delta x_k \perp u, \\ x_{k+1} = x_k + \Delta x_k, \text{ and normalize when necessary} \end{array}\right. . \tag{2.16}$$

It can be shown that the exact solution of the correction equation is

$$\Delta x_k = \frac{T^{-1}(\rho_k)T'(\rho_k)x_k}{u^*T^{-1}(\rho_k)T'(\rho_k)x_k} - x_k$$

so that $x_k + \Delta x_k = T^{-1}(\rho_k)T'(\rho_x)x_k$ up to a scaling factor. Therefore, this variant of JD is mathematically equivalent to RFI, provided $y_kT'(\rho_k)x_k \neq 0$ so that $\Pi_k^{(1)}$ is well-defined and $u^*T^{-1}(\rho_k)T'(\rho_x)x_k \neq 0$.

In practice, to enhance the robustness and the rate of convergence, JD usually works with a search subspace of variable dimension for eigenvector approximations, and in this case it is referred to as the full JD method. In this paper, we restrict our discussion to the local convergence of single-vector JD, which can be used as a worst-case estimate of the convergence rates of full JD.

2.4. Convergence of Newton's method near singular roots. We end this section by reviewing the local convergence of Newton's method for a nonlinear system of algebraic equations $F(z) = 0$ towards a root z^* for which the Jacobian $F'(z^*)$ is singular. The typical convergence behavior can be roughly described as follows. The whole space for the variable z can be decomposed as a direct sum of the null space $\mathcal{N}_1$ of $F'(z^*)$ and an appropriate complementary space $\mathcal{M}_1$. When Newton's method converges towards z^*, the component of the iterate error in $\mathcal{N}_1$ converges *linearly*, whereas the error component in $\mathcal{M}_1$ converges quadratically; see, e.g., [6, 7, 8]. To prepare for the convergence analysis of inverse iteration towards degenerate eigenvalues, we need to review some results from [8].

Let $\mathcal{N}_1 = \text{null}(F'(z^*))$, $\mathcal{M}_2 = \text{range}(F'(z^*))$, so that $\text{codim}(\mathcal{M}_2) = \dim(\mathcal{N}_1)$. We choose complementary subspaces $\mathcal{M}_1$, $\mathcal{N}_2$ such that $\mathbb{C}^{n+1} = \mathcal{N}_1 \oplus \mathcal{M}_1 = \mathcal{N}_2 \oplus \mathcal{M}_2$. Define $P_{\mathcal{N}_i}$ as the projections onto $\mathcal{N}_i$ along $\mathcal{M}_i$, and $P_{\mathcal{M}_i} = I - P_{\mathcal{N}_i}$. Given these subspaces, the Jacobian $F'(z)$ can be decomposed as

$$F'(z) = A_F(z) + B_F(z) + C_F(z) + D_F(z),$$

where

$$\begin{aligned} A_F(z) &= P_{\mathcal{M}_2}F'(z)P_{\mathcal{M}_1}, \quad B_F(z) = P_{\mathcal{M}_2}F'(z)P_{\mathcal{N}_1} \\ C_F(z) &= P_{\mathcal{N}_2}F'(z)P_{\mathcal{M}_1}, \quad D_F(z) = P_{\mathcal{N}_2}F'(z)P_{\mathcal{N}_1}. \end{aligned} \tag{2.17}$$

Let $A_{F^*} = P_{\mathcal{M}_2}A_F(z^*)P_{\mathcal{M}_1}$, which is a bijection when considered as an operator from $\mathcal{M}_1$ into $\mathcal{M}_2$. The conditions for the nonsingularity of $F'(z)$ are described as follows.

PROPOSITION 2.4. *Let z be a candidate Newton iterate and $e_z = z - z^*$ be the iterate error. For $z \in S_\delta \equiv \{z : \|e_z\| \leq \delta\}$ with a sufficiently small $\delta > 0$, $F'(z)$ is nonsingular if and only if the Schur complement*

$$S_F(z) : \mathcal{N}_1 \to \mathcal{N}_2 \equiv D_F(z) - C_F(z)A_F^{-1}(z)B_F(z) \tag{2.18}$$

is nonsingular. In this case, we have

$$\begin{aligned} F'(z)^{-1} &= \big(A_F(z) + B_F(z) + C_F(z) + D_F(z)\big)^{-1} \\ &= P_{\mathcal{M}_1}\big(A_F^{-1}(z) + A_F^{-1}(z)B_F(z)S_F^{-1}(z)C_F(z)A_F^{-1}(z)\big)P_{\mathcal{M}_2} \\ &\quad -P_{\mathcal{M}_1}A_F^{-1}(z)B_F(z)S_F^{-1}(z)P_{\mathcal{N}_2} \\ &\quad -P_{\mathcal{N}_1}S_F^{-1}(z)C_F(z)A_F^{-1}(z)P_{\mathcal{M}_2} + P_{\mathcal{N}_1}S_F^{-1}(z)P_{\mathcal{N}_2}. \end{aligned} \tag{2.19}$$

The convergence of Newton's method can be explored by studying each term in (2.19). To this end, note that Taylor expansions of the terms in (2.17) at z^*, i.e., the restrictions of the Jacobian $F'(z)$ onto $\mathcal{M}_i$ and $\mathcal{N}_i$ $(i = 1, 2)$, are as follows:

$$
\begin{aligned}
A_F(z) &= A_{F^*} + \sum_{j=a}^{n} A_{(j)}(z) + \mathcal{O}_{n+1}(e_z), \\
B_F(z) &= \sum_{j=b}^{n} B_{(j)}(z) + \mathcal{O}_{n+1}(e_z), \\
C_F(z) &= \sum_{j=c}^{n} C_{(j)}(z) + \mathcal{O}_{n+1}(e_z), \\
D_F(z) &= \sum_{j=d}^{n} D_{(j)}(z) + \mathcal{O}_{n+1}(e_z),
\end{aligned} \tag{2.20}
$$

where

$$
\begin{aligned}
A_{(j)}(z) &= \frac{1}{j!} P_{\mathcal{M}_2} F^{(j+1)}(z^*)(e_z^j, P_{\mathcal{M}_1}\cdot), \\
B_{(j)}(z) &= \frac{1}{j!} P_{\mathcal{M}_2} F^{(j+1)}(z^*)(e_z^j, P_{\mathcal{N}_1}\cdot), \\
C_{(j)}(z) &= \frac{1}{j!} P_{\mathcal{N}_2} F^{(j+1)}(z^*)(e_z^j, P_{\mathcal{M}_1}\cdot), \quad \text{and} \\
D_{(j)}(z) &= \frac{1}{j!} P_{\mathcal{N}_2} F^{(j+1)}(z^*)(e_z^j, P_{\mathcal{N}_1}\cdot)
\end{aligned} \tag{2.21}
$$

are square matrices. Here, $F^{(j+1)}(z^*)(\cdot, \cdots, \cdot)$ stands for the $(j+1)$st derivative of F at z^* (a multilinear form (tensor) with $j+1$ arguments), and e_z^j means that the first j arguments of $F^{(j+1)}$ are all e_z. The values $j = a, b, c, d > 0$ in (2.20) are the smallest integers for which the *vectors* $A_{(j)}(z)e_z$, $B_{(j)}(z)e_z$, $C_{(j)}(z)e_z$, and $D_{(j)}(z)e_z$, respectively, are nonzero. In addition, let $j = \bar{a}, \bar{b}, \bar{c}, \bar{d}$ be the smallest integers for which the *matrices* $A_{(j)}(z)$, $B_{(j)}(z)$, $C_{(j)}(z)$ and $D_{(j)}(z)$ are nonzero. Obviously, we have $\bar{a} \le a, \bar{b} \le b, \bar{c} \le c$ and $\bar{d} \le d$.

With the above notation and definitions, a major convergence result of the standard Newton's method near singular points developed in [8] is summarized as follows.

THEOREM 2.5 (Theorem 5.9 in [8]). *Define the operator*

$$
\widetilde{D}_{(j)} = \frac{1}{j!} P_{\mathcal{N}_2} F^{(j+1)}(z^*)((P_{\mathcal{N}_1} e_z)^j, P_{\mathcal{N}_1}\cdot),
$$

and $j = \widetilde{d}$ be the smallest integer for which $\widetilde{D}_{(j)} \not\equiv 0$. Let $e_z = z - z^*$ be the error of z, and assume that $\bar{d} = \widetilde{d} \le c$ and $\widetilde{D}_{(\bar{d})}$ is nonsingular for all $P_{\mathcal{N}_1} e_z \neq 0$. Define $\ell = \min(a, b, c, d)$, and let z_0 be the initial Newton iterate. Then, for sufficiently small $\delta > 0$ and $\theta > 0$, $F'(z_0)$ is nonsingular for all

$$
z_0 \in W(\delta, \theta) \equiv \{ z : 0 < \|e_z\| \le \delta,\ \|P_{\mathcal{M}_1} e_z\| \le \theta \|P_{\mathcal{N}_1} e_z\| \},
$$

all subsequent Newton iterates remain in $W(\delta, \theta)$; in addition, $z_k \to z^*$ with

$$
\|P_{\mathcal{M}_1}(z_k - z^*)\| \le C \|P_{\mathcal{M}_1}(z_{k-1} - z^*)\|^{\ell+1}
$$

for some constant $C > 0$ independent of k, and

$$\lim_{k\to\infty} \frac{\|P_{\mathcal{N}_1}(z_k - z^*)\|}{\|P_{\mathcal{N}_1}(z_{k-1} - z^*)\|} = \frac{\bar{d}}{\bar{d}+1}.$$

Theorem 2.5 states that under certain assumptions, as Newton's method converges towards z^* for which $F'(z^*)$ is singular, the error component lying in $\mathcal{M}_1$ converges at least quadratically, whereas the error component lying in $\mathcal{N}_1$ converges only linearly. This observation will be used directly in Sections 3 and 4 to show the quadratic and linear convergence of inverse iteration, respectively, towards a semi-simple and a defective eigenpair.

3. Convergence for semi-simple eigenvalues. In this section, we study the local convergence of Newton-like methods for a semi-simple eigenvalue of the nonlinear algebraic eigenvalue problem (1.1). As we shall see, the Jacobian of the augmented system (2.12) is singular at a semi-simple eigenpair, and the convergence theory of Newton's method near singular roots indicates that the algorithm generally converges only linearly. However, we show that the singularity of the Jacobian does not hamper the quadratic convergence of Newton's method towards semi-simple eigenvalues; in addition, Rayleigh functional iteration converges at least quadratically, and it converges cubically for locally symmetric problems. These convergence results are very similar to those for simple eigenvalues; see, e.g., [25, 29].

3.1. Inverse iteration. Assume that (λ, v) is a semi-simple eigenpair of the holomorphic matrix pencil $T(\cdot)$, and $\varphi_1, \ldots, \varphi_J$ and $\psi_1, \ldots, \psi_J$ are the corresponding left and right eigenvectors. Since $\dim(\operatorname{null} T(\lambda)) = J$, there exists a singular value decomposition of $T(\lambda)$ of the following form

$$Y^* T(\lambda) X = \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_{n-J} \end{bmatrix},$$

where $X = [X_J \ X_{n-J}]$ and $Y = [Y_J \ Y_{n-J}]$ are unitary matrices, $X_J \in \mathbb{C}^{n\times J}$ and $Y_J \in \mathbb{C}^{n\times J}$ have orthonormal columns that form a basis of $\operatorname{span}\{\varphi_1, \ldots, \varphi_J\}$ and $\operatorname{span}\{\psi_1, \ldots, \psi_J\}$, respectively, and Σ_{n-J} is a diagonal matrix of positive singular values of $T(\lambda)$. Therefore there exist nonsingular matrices $K_J, M_J \in \mathbb{C}^{J\times J}$ such that $X_J = [\varphi_1 \ \ldots \ \varphi_J]K_J$ and $Y_J = [\psi_1 \ \ldots \ \psi_J]M_J$. Since $v \in \operatorname{span}\{\varphi_1, \ldots, \varphi_J\}$, we can write $v = [\varphi_1 \ \ldots \ \varphi_J]d_v$ for some nonzero $d_v \in \mathbb{C}^J$. It follows from (2.1) that

$$Y_J^* T'(\lambda) v = M_J^* [\psi_1 \ \ldots \ \psi_J]^* T'(\lambda) [\varphi_1 \ \ldots \ \varphi_J] d_v = M_J^* d_v,$$

and consequently

$$\begin{aligned} (3.1) \qquad & \begin{bmatrix} Y^* & \\ & 1 \end{bmatrix} \begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix} \begin{bmatrix} X & \\ & 1 \end{bmatrix} = \begin{bmatrix} Y^*T(\lambda)X & Y^*T'(\lambda)v \\ u^*X & 0 \end{bmatrix} \\ & = \begin{bmatrix} 0 & 0 & M_J^* d_v \\ 0 & \Sigma_{n-J} & Y_{n-J}^* T'(\lambda) v \\ u^*X_J & u^*X_{n-J} & 0 \end{bmatrix}. \end{aligned}$$

Let $h = [h_a^* \ h_b^* \ \bar{h}_c]^*$ be a vector in the null space of the above square matrix, where $h_a \in \mathbb{C}^J$, $h_b \in \mathbb{C}^{n-J}$ and $h_c \in \mathbb{C}$. Then

$$\begin{bmatrix} 0 & 0 & M_J^* d_v \\ 0 & \Sigma_{n-J} & Y_{n-J}^* T'(\lambda) v \\ u^*X_J & u^*X_{n-J} & 0 \end{bmatrix} \begin{bmatrix} h_a \\ h_b \\ h_c \end{bmatrix} = \begin{bmatrix} M_J^* d_v h_c \\ \Sigma_{n-J} h_b + Y_{n-J}^* T'(\lambda) v h_c \\ u^*X_J h_a + u^*X_{n-J} h_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

In the first J rows, since M_J is nonsingular and $d_v \neq 0$, we have $M_J^* d_v \neq 0$, and therefore $h_c = 0$. The next $n-J$ rows is thus simplified as $\Sigma_{n-J} h_b$, and since Σ_{n-J} is diagonal with all nonzero entries, we have $h_b = 0$, and the last row is equivalent to $u^* X_J h_a = 0$. Now, since u with $u^* v = 1$ specifies the scaling of $v = [\varphi_1 \ \dots \ \varphi_J] d_v$ in the desired eigenspace range(X_J), we have $u^* X_J \neq 0$. Without loss of generality, assume that $u^* X_J = [\eta_1 \ \dots \ \eta_J]$ where $\eta_J \neq 0$. Then we can determine h_a and h.

$$h = \begin{bmatrix} h_a \\ h_b \\ h_c \end{bmatrix} \in \text{span} \left\{ \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ -\frac{\eta_1}{\eta_J} \\ 0_{n-J+1} \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \\ -\frac{\eta_2}{\eta_J} \\ 0_{n-J+1} \end{bmatrix}, \dots, \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ -\frac{\eta_{J-1}}{\eta_J} \\ 0_{n-J+1} \end{bmatrix} \right\}.$$

We see from (3.1) that the null space of the Jacobian $\begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix}$ can be obtained by premultiplying h by $\begin{bmatrix} X & \\ & 1 \end{bmatrix}$.

$$\begin{aligned} (3.2) \quad \mathcal{N}_1 &\equiv \text{null}\left(\begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix} \right) \\ &= \begin{bmatrix} X & \\ & 1 \end{bmatrix} \text{span} \left\{ \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ -\frac{\eta_1}{\eta_J} \\ 0_{n-J+1} \end{bmatrix}, \dots, \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ -\frac{\eta_{J-1}}{\eta_J} \\ 0_{n-J+1} \end{bmatrix} \right\} \\ &= \text{span} \left\{ \begin{bmatrix} Xe_1 - \frac{\eta_1}{\eta_J} Xe_J \\ 0 \end{bmatrix}, \begin{bmatrix} Xe_2 - \frac{\eta_2}{\eta_J} Xe_J \\ 0 \end{bmatrix}, \dots, \begin{bmatrix} Xe_{J-1} - \frac{\eta_{J-1}}{\eta_J} Xe_J \\ 0 \end{bmatrix} \right\} \\ &\subset \text{span} \left\{ \begin{bmatrix} \varphi_1 \\ 0 \end{bmatrix}, \dots, \begin{bmatrix} \varphi_J \\ 0 \end{bmatrix} \right\}, \end{aligned}$$

where $\dim(\mathcal{N}_1) = J - 1$ $(J \geq 2)$.

The special structure of the null space $\mathcal{N}_1$ indicates that the convergence of Newton's method towards the semi-simple eigenvalue and the corresponding *eigenspace* (instead of the eigenvector v) is quadratic. To see this, define the space

$$\mathcal{M}_1 = \mathcal{M}_{1\alpha} \oplus \mathcal{M}_{1\beta} = \text{span} \left\{ \begin{bmatrix} Xe_J \\ 0 \end{bmatrix} \right\} \oplus \text{range} \left(\begin{bmatrix} X_{n-J} & \\ & 1 \end{bmatrix} \right),$$

so that $\dim(\mathcal{M}_1) = n - J + 2$. Therefore

$$\begin{aligned} \mathbb{C}^{n+1} &= \text{span} \left\{ \begin{bmatrix} Xe_1 - \frac{\eta_1}{\eta_J} Xe_J \\ 0 \end{bmatrix}, \dots, \begin{bmatrix} Xe_{J-1} - \frac{\eta_{J-1}}{\eta_J} Xe_J \\ 0 \end{bmatrix} \right\} \\ &\qquad \oplus \left(\text{span} \left\{ \begin{bmatrix} Xe_J \\ 0 \end{bmatrix} \right\} \oplus \text{range} \left(\begin{bmatrix} X_{n-J} & \\ & 1 \end{bmatrix} \right) \right) \\ &= \mathcal{N}_1 \oplus (\mathcal{M}_{1\alpha} \oplus \mathcal{M}_{1\beta}) = \mathcal{N}_1 \oplus \mathcal{M}_1. \end{aligned}$$

Let $\mathcal{P}_{\mathcal{N}_1}$ be the projector onto $\mathcal{N}_1$ along $\mathcal{M}_1$, $\mathcal{P}_{\mathcal{M}_1} = I - \mathcal{P}_{\mathcal{N}_1}$, and $e_k = \begin{bmatrix} x_k \\ \mu_k \end{bmatrix} - \begin{bmatrix} v \\ \lambda \end{bmatrix}$ be the error between the Newton iterate and the *particular eigenpair* (λ, v) in the kth iteration. We know from Theorem 2.5 that $\|\mathcal{P}_{\mathcal{N}_1}(e_k)\|$ and $\|\mathcal{P}_{\mathcal{M}_1}(e_k)\|$, respectively, converge to zero linearly and quadratically. Therefore Newton's method converges towards the *particular eigenpair* (λ, v) linearly.

Fortunately, the linear convergence of Newton's method towards (λ, v) does not affect its quadratic convergence towards λ and the desired *eigenspace*. The key observation is that the error between the Newton iterate and the eigenvalue together with its eigenspace lies in $\mathcal{M}_1$, and $\|\mathcal{P}_{\mathcal{M}_1}(e_k)\|$ converges quadratically. In fact, the eigenspace approximation error in range $\left(\begin{bmatrix} X_{n-J} \\ 0 \end{bmatrix}\right)$ together with the eigenvalue approximation error in span $\left\{\begin{bmatrix} 0 \\ 1 \end{bmatrix}\right\}$ can be represented by $\mathcal{P}_{\mathcal{M}_{1\beta}}(e_k)$, the projection of e_k onto $\mathcal{M}_{1\beta} = \text{range}\left(\begin{bmatrix} X_{n-J} & \\ & 1 \end{bmatrix}\right)$ along $\mathcal{N}_1 \oplus \mathcal{M}_{1\alpha} = \text{span}\left\{\begin{bmatrix} \varphi_1 \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} \varphi_J \\ 0 \end{bmatrix}\right\}$. Therefore, $\mathcal{P}_{\mathcal{M}_{1\beta}}(e_k)$, instead of $\mathcal{P}_{\mathcal{N}_1}(e_k)$, represents the error between the Newton iterate and the space $\mathcal{E} = \text{span}\left\{\begin{bmatrix} \varphi_1 \\ \lambda \end{bmatrix}, \ldots, \begin{bmatrix} \varphi_J \\ \lambda \end{bmatrix}\right\}$ spanned by all valid candidate eigenpairs. In addition, (3.2) shows that any vector lying in $\mathcal{N}_1$ can be represented as the difference between two candidate eigenpairs, and thus $\mathcal{P}_{\mathcal{N}_1}(e_k)$ bears no connection to the error between the Newton iterate and $\mathcal{E}$ spanned by all candidate eigenpairs. Since $\mathcal{M}_{1\beta} \subset \mathcal{M}_1$, the quadratic convergence of Newton's method towards the semi-simple λ and its eigenspace (represented by $\mathcal{E}$) is established from the quadratic convergence of $\|\mathcal{P}_{\mathcal{M}_1}(e_k)\|$. This result is summarized as follows.

THEOREM 3.1. *Let λ be a semi-simple eigenvalue of the holomorphic operator $T(\cdot) : U \to \mathbb{C}^{n\times n}$, and $\varphi_1, \ldots, \varphi_J$ be the corresponding right eigenvectors. Let (μ_0, x_0) be a right eigenpair approximation such that $|\mu_0 - \lambda|$ and $\angle(x_0, \text{span}\{\varphi_1, \ldots, \varphi_J\})$ are sufficiently small. Assume that the conditions in* Theorem 2.5 *hold. Then inverse iteration* (2.14) *converges towards λ together with its eigenspace quadratically.*

3.2. Numerical experiments for inverse iteration. In this section, we provide numerical results illustrating the locally quadratic convergence of inverse iteration for semi-simple eigenvalues. The experiments are performed on five benchmark problems, one from the MatrixMarket [16], two from the NLEVP toolbox [2], and two constructed artificially. A description of these problems is given in Table 3.1.

problem	source	type	size	eigenvalue	multiplicity	local symm.
*tols*1090	MM	lep	1090	-12.098	200	real unsymm.
plasma_drift	NLEVP	pep	128	$10.004129-0.19324032i$	2	cplx unsymm.
schrödinger	NLEVP	qep	1998	$-0.33111181+0.24495497i$	2	cplx symm.
ss_art_symm	artificial	nep	256	0	5	real symm.
ss_art_unsymm	artificial	nep	256	0	5	real unsymm.

TABLE 3.1
Description of the test problems for semi-simple eigenvalues

For example, the problem *tols*1090 taken from the MatrixMarket (MM) is a linear eigenvalue problem (lep), defined by a matrix $A \in \mathbb{R}^{1090\times 1090}$; it has a semi-simple eigenvalue $\lambda = -12.098$ of multiplicity 200, and the matrix $T(\lambda) = \lambda I - A$ is real unsymmetric (local symmetry). Similarly, *plasma_drift* and *schrödinger* taken from

NLEVP, respectively, are a polynomial eigenvalue problem (pep) of degree 3 and a quadratic eigenvalue problem (qep); they both have a semi-simple eigenvalue λ of multiplicity 2, and $T(\lambda)$ is complex unsymmetric and complex symmetric, respectively. The two artificial problems are both truly nonlinear eigenvalue problems (nep), where $T(\mu)$ cannot be represented as a polynomial of μ; specifically,

$$T_{symm}(\mu) = G_A^* D(\mu) G_A \quad \text{for} \quad \text{“}ss\_art\_symm\text{”}, \quad \text{and} \tag{3.3}$$
$$T_{unsymm}(\mu) = G_A^* D(\mu) G_B \quad \text{for} \quad \text{“}ss\_art\_unsymm\text{”},$$

where $D(\mu) = \mathrm{diag}([e^\mu - 1;\ 2\sin\mu;\ -5\ln(1+\mu);\ 8\mu;\ \tan^{-1}(\mu);\ c_0 + c_1\mu + c_2\mu^2])$, $c_i \in \mathbb{R}^{251}\,(i = 0, 1, 2)$ and $G_A, G_B \in \mathbb{R}^{256\times 256}$ generated by MATLAB's function `randn` are random matrices whose entries follow the standard normal distribution. Both artificial problems have a semi-simple eigenvalue $\lambda = 0$ of multiplicity 5.

To test the local convergence of inverse iteration for these problems, we first construct an initial eigenvector approximation using the MATLAB commands

$$\texttt{x\_0} = \texttt{v} * \texttt{cos}(\texttt{err\_phi}) + \texttt{g} * \texttt{sin}(\texttt{err\_phi}); \tag{3.4}$$

where v is a normalized eigenvector corresponding to the desired eigenvalue of the given problem, g is a normalized random vector that has been orthogonalized against v, and *err_phi* is the error angle $\angle(x_0, v)$. An appropriate value for *err_phi* is obtained by trial and error, such that quadratic convergence of inverse iteration can be clearly observed. The initial eigenvalue approximation μ_0 is defined as the value of the one-sided Rayleigh functional $\rho_F(x_0; T, y)$ where the auxiliary vector $y = T'(\lambda)v$, and therefore $|\mu_0 - \lambda| = \mathcal{O}\left(\angle(x_0, v)\right)$.

To estimate the convergence rate of inverse iteration, we monitor how quickly the eigenresidual norm $e_k := \|T(\mu_k)x_k\|$ decreases as the algorithm proceeds. The residual norm is a natural measure of the eigenpair approximation error of (μ_k, x_k), and it can be evaluated at little cost. For all the test problems, it is easy to see that inverse iteration converges at least superlinearly. Nevertheless, our goal in this section is to show that the order of convergence ℓ of this algorithm is exactly 2, and the standard criterion $\|e_{k+1}\|/\|e_k\|^\ell \le C$ may not be very descriptive for this purpose. For example, if $e_0 = 10^{-2}$, $e_1 = 10^{-5}$ and $e_2 = 10^{-12}$, it is then difficult to tell if the convergence is quadratic, superquadratic or cubic, due to the very small number of iterations for which the standard criterion holds.

We now discuss an alternative approach to estimate ℓ in a more descriptive manner. First, we generate a *sequence* of initial approximations $(\mu_0^{(j)}, x_0^{(j)})$, such that $\angle(v, x_0^{(j+1)}) = \frac{1}{2}\angle(v, x_0^{(j)})$, and thus $|\mu_0^{(j+1)} - \lambda| \approx \frac{1}{2}|\mu_0^{(j)} - \lambda|$ since the value of the Rayleigh functional $\mu_0^{(j)} = \rho_F(x_0^{(j)}; T, y)$ satisfies $|\mu_0^{(j)} - \lambda| = \mathcal{O}\big(\angle(x_0^{(j)}, v)\big)$. It can be shown that $e_0^{(j+1)} = \|T(\mu_0^{(j+1)})x_0^{(j+1)}\| \approx \frac{1}{2}e_0^{(j)} = \frac{1}{2}\|T(\mu_0^{(j)})x_0^{(j)}\|$. We then apply one step of inverse iteration to generate a sequence of new iterates $(\mu_1^{(j)}, x_1^{(j)})$, for which $e_1^{(j+1)} = \left(\frac{1}{2}\right)^\ell e_1^{(j)}$ holds, and an estimate of ℓ can be obtained. This approach is more descriptive for our purpose, because a relatively large number of initial approximations can be generated, for which the algorithm exhibits the ℓth order of convergence for at least one iteration.

The estimated order of convergence of inverse iteration is summarized in Table 3.2. To explain the results, take for instance the problem *tols*1090. We generated 20 initial approximations $(\mu_0^{(j)}, x_0^{(j)})$ $(j = 1, 2, \ldots, 20)$, where $\angle(x_0^{(1)}, v) = 10^{-2}$ and $\angle(x_0^{(j+1)}, v) = \frac{1}{2}\angle(x_0^{(j)}, v)$. The estimates of the order of convergence ℓ are obtained

by applying the least-squares line formula to $\left(\log e_0^{(j)}, \log e_1^{(j)}\right)$. As one can see, the estimated values of ℓ are very close to 2, indicating that inverse iteration converges quadratically, independent of the local symmetry; see Theorem 3.1.

problem	$\angle(x_0^{(1)}, v)$	# init. approx.	estimated ℓ
*tols*1090	10^{-2}	20	2.022
plasma_drift	2×10^{-1}	20	2.002
schrödinger	10^{-4}	13	1.979
ss_art_symm	2×10^{-2}	16	2.008
ss_art_unsymm	2×10^{-2}	16	1.983

TABLE 3.2
Estimated order of convergence for inverse iteration

3.3. Rayleigh functional iteration and single-vector JD. We see that a semi-simple eigenvalue is a class of degenerate eigenvalue for which Newton's method exhibit the same order of convergence as that for simple eigenvalues. In fact, we can take a step further and show that Rayleigh functional iteration (RFI), a variant of Newton's method which approximates eigenvalues in a different manner, converges cubically towards a semi-simple eigenvalue λ if the problem is locally symmetric, i.e., if $T(\lambda)$ is (skew) real/complex symmetric or (skew) Hermitian. In this case, note that the right and the left eigenvectors satisfy $\varphi_j = \psi_j$ or $\varphi_j = \overline{\psi}_j$ $(j = 1, \ldots, J)$, so that a left eigenvector approximation can be obtained in each iteration without additional computational cost.

We now present the local convergence analysis of RFI. First, note that for any $v = \sum_{j=1}^{J} \alpha_j \varphi_j$ such that $T(\lambda)v = 0$, we have

$$\sum_{k=1}^{J} \left(\psi_k^* T'(\lambda) v\right) \varphi_k = \sum_{k=1}^{J} \left(\sum_{j=1}^{J} \alpha_j \left(\psi_k^* T'(\lambda) \varphi_j\right) \right) \varphi_k = \sum_{k=1}^{J} \alpha_k \varphi_k = v. \tag{3.5}$$

Note from (2.2) that for such v, we have $Q(\lambda)T'(\lambda)v \in \operatorname{span}\{\varphi_1, \ldots, \varphi_J\}$ where both $Q(\mu)$ and $T'(\mu)$ are holomorphic in a neighborhood of λ; that is, there exists some constant α such that

$$Q(\lambda)T'(\lambda)v = \alpha\widetilde{v} \quad \text{with} \quad \widetilde{v} \in \operatorname{span}\{\varphi_1, \ldots, \varphi_J\}. \tag{3.6}$$

In the following derivation, let $\rho = \rho_F(x; T, y)$ be the Rayleigh functional value corresponding to x and an auxiliary vector q. To prepare for the analysis, we also need decompositions of the following vectors

$$Q(\lambda)T'(\lambda)g = \gamma_1(c_1 v_1 + s_1 g_1), \tag{3.7}$$

$$Q'(\lambda)T'(\rho)x = \gamma_2(c_2 v_2 + s_2 g_2), \quad \text{and} \tag{3.8}$$

$$Q(\rho)T''(\lambda)x = \gamma_3(c_3 v_3 + s_3 g_3), \tag{3.9}$$

which can be obtained by substituting the left-hand sides in (3.7)–(3.9), respectively, for x in (2.5). Therefore $v_j \in \operatorname{span}\{\varphi_1, \ldots, \varphi_J\}$ and

$$T'(\lambda)g_j \perp \operatorname{span}\{\psi_1, \ldots, \psi_J\} \tag{3.10}$$

for $j = 1, 2, 3$; see (2.5)–(2.7). Without loss of generality, assume that the right eigenvector approximation x has a unit generalized norm, i.e., $\gamma = 1$; see (2.5) and

(2.6). Assuming that ρ is in a neighborhood of λ in which F is analytic, the generalized norms γ_j of these vectors are bounded above by $\mathcal{O}(1)$. It follows that the new unnormalized eigenvector approximation p computed by RFI is

$$\begin{aligned}
p = T^{-1}(\rho)T'(\rho)x &= \frac{1}{\rho-\lambda}\sum_{k=1}^{J}\left(\psi_k^* T'(\rho)x\right)\varphi_k + Q(\rho)T'(\rho)x \\
&= \frac{1}{\rho-\lambda}\sum_{k=1}^{J}\psi_k^*\left(T'(\lambda)(cv+sg) + (\rho-\lambda)T''(\lambda)x + \frac{(\rho-\lambda)^2}{2}T'''(\lambda)x\right)\varphi_k + \\
&\qquad Q(\lambda)T'(\lambda)(cv+sg) + (\rho-\lambda)\left(Q'(\lambda)T'(\rho) + Q(\rho)T''(\lambda)\right)x + \mathcal{O}\left(|\rho-\lambda|^2\right) \\
&= \frac{cv}{\rho-\lambda} + \sum_{k=1}^{J}\left(\psi_k^* T''(\lambda)x + \frac{\rho-\lambda}{2}\psi_k^* T'''(\lambda)x\right)\varphi_k + c\alpha\widetilde{v} + sQ(\lambda)T'(\lambda)g + \\
&\qquad (\rho-\lambda)\left(Q'(\lambda)T'(\rho) + Q(\rho)T''(\lambda)\right)x + \mathcal{O}\left(|\rho-\lambda|^2\right) \text{ (see (2.7),(3.5) and (3.6))} \\
&= \frac{cv}{\rho-\lambda} + \sum_{k=1}^{J}\eta_k\varphi_k + c\alpha\widetilde{v} + s\gamma_1 c_1 v_1 + (\rho-\lambda)(\gamma_2 c_2 v_2 + \gamma_3 c_3 v_3) + \\
&\qquad s\gamma_1 s_1 g_1 + (\rho-\lambda)(\gamma_2 s_2 g_2 + \gamma_3 s_2 g_3) + \mathcal{O}\left(|\rho-\lambda|^2\right) \text{ (see (3.7)–(3.9))} \\
&= \widehat{v}_p + \widehat{g}_p + \mathcal{O}\left(|\rho-\lambda|^2\right),
\end{aligned}$$

where

$$\begin{aligned}
\widehat{v}_p &= \frac{cv}{\rho-\lambda} + \sum_{k=1}^{J}\eta_k\varphi_k + c\alpha\widetilde{v} + s\gamma_1 c_1 v_1 + (\rho-\lambda)(\gamma_2 c_2 v_2 + \gamma_3 c_3 v_3), \\
\eta_k &= \psi_k^* T''(\lambda)x + \frac{\rho-\lambda}{2}\psi_k^* T'''(\lambda)x, \quad \text{and} \\
\widehat{g}_p &= s\gamma_1 s_1 g_1 + (\rho-\lambda)(\gamma_2 s_2 g_2 + \gamma_3 s_2 g_3),
\end{aligned}$$

so that $\widehat{v}_p \in \operatorname{span}\{\varphi_1,\ldots,\varphi_J\}$ and $T'(\lambda)\widehat{g}_p \perp \operatorname{span}\{\psi_1,\ldots,\psi_J\}$.

The convergence rates of RFI can be obtained by studying the error angle $\angle(p,\widehat{v}_p)$. Recall that $\rho = \rho_F(x;T,y)$ is the Rayleigh functional value such that $y^*T(\rho)x = 0$. Suppose that x is a good right eigenvector approximation for which the generalized sine s is sufficiently small, then $|\rho-\lambda| = \mathcal{O}(s^2)$ if $T(\cdot)$ is locally symmetric and $|\rho-\lambda| = \mathcal{O}(s)$ otherwise; see Theorem 5 in [26]. In both cases, it is easy to see that $(\rho-\lambda)^{-1}cv$ is the unique dominant term in $\widehat{v}_p$, and $\|\widehat{v}_p\| = \mathcal{O}(|\rho-\lambda|^{-1})$; in addition, $\|\widehat{g}_p\| = \mathcal{O}(s) + \mathcal{O}(|\rho-\lambda|) = \mathcal{O}(s)$. Following the discussion of the error angle $\angle(x,v)$ (see (2.5) and (2.6)), we see that the generalized tangent of the error angle $\angle(p,\widehat{v}_p)$ is bounded above by a quantity proportional to the ratio between the magnitude of the error component $\widehat{g}_p$ and that of the eigenvector component $\widehat{v}_p$. That is,

$$\begin{aligned}
\operatorname{gtan}(p,\widehat{v}_p) &\le \mathcal{O}\left(\frac{\|\widehat{g}_p\| + \mathcal{O}(|\rho-\lambda|^2)}{\|\widehat{v}_p\| - \mathcal{O}(|\rho-\lambda|^2)}\right) = \mathcal{O}(|\rho-\lambda|s) \\
&= \begin{cases} \mathcal{O}(s^3) & \text{if } T(\cdot) \text{ is locally symmetric} \\ \mathcal{O}(s^2) & \text{otherwise} \end{cases}.
\end{aligned}$$

In other words, the convergence rates of RFI towards semi-simple and simple eigenvalues are identical. This conclusion also holds for the single-vector JD method (2.16) because it is mathematically equivalent to RFI. The result is summarized in the following theorem.

THEOREM 3.2. *Let λ be a semi-simple eigenvalue of the holomorphic operator $T(\cdot) : U \to \mathbb{C}^{n\times n}$, and $x_0 = \gamma(c_0 v + s_0 g)$ be a corresponding initial right eigenvector approximation with a sufficiently small error angle $\angle(x_0, v)$. Then RFI* (2.15) *and single-vector JD* (2.16) *converge towards λ and its eigenspace at least quadratically or at least cubically for locally nonsymmetric or symmetric problems, respectively.*

3.4. Numerical experiments for RFI and JD. In this section, we test the convergence of RFI and single-vector JD on the five problems with semi-simple eigenvalues introduced in Section 3.2. We follow the same approach used for inverse iteration to estimate the order of convergence for RFI, with the only difference in the generation of the initial eigenvalue approximations $\mu_0^{(j)}$. To achieve the maximum order of convergence for RFI, as discussed in Section 3.3, we use the two-sided Rayleigh functional whenever the local symmetry exists; that is, for *schrödinger* and *ss_art_symm* (see Table 3.1), we choose $y = \mathrm{conj}(x_0^{(j)})$ and $y = x_0^{(j)}$, respectively, and let $\mu_0^{(j)} = \rho_F(x_0^{(j)}; T, y)$, such that $|\mu_0^{(j)} - \lambda| = \mathcal{O}\big(\angle(x_0^{(j)}, v)^2\big)$. As a result, RFI converges at least cubically for these problems.

Table 3.3 presents the estimated order of convergence for RFI. The results also hold for single-vector JD because the two algorithms are mathematically equivalent. We see that RFI converges quadratically for the three problems without local symmetry, and it converges cubically for the two problems with local symmetry (see the numbers in bold in Table 3.3). All these results are consistent with Theorem 3.2.

problem	$\angle(x_0^{(1)}, v)$	# init. approx.	estimated ℓ
*tols*1090	10^{-6}	16	2.013
plasma_drift	5×10^{-4}	11	2.012
schrödinger	5×10^{-4}	10	**2.972**
ss_art_symm	2×10^{-2}	12	**3.006**
ss_art_unsymm	2×10^{-2}	17	1.997

TABLE 3.3
Estimated order of convergence for RFI/JD

4. Convergence for defective eigenvalues. We see in Section 3 that Newton-like methods converge towards semi-simple eigenvalues at least quadratically. In this section, we study the computation of defective eigenvalues, which is naturally more challenging. We show that the local convergence of the standard Newton-like methods towards a defective eigenpair is generally only linear. Then we propose an accelerated inverse iteration, and show that it converges quadratically under certain assumptions, where in each iteration two linear systems need to be solved. This convergence rate is also referred to as superlinear convergence of order $\sqrt{2}$. This algorithm is inspired by an accelerated Newton's method for solving a general nonlinear system for a singular root [8]. In addition, we present an accelerated single-vector Jacobi-Davidson method, which also converges quadratically in this case.

4.1. Inverse iteration. The proof of the linear convergence of inverse iteration for defective eigenvalues is similar to that for semi-simple eigenvalues. Let λ be a defective eigenvalue of $T(\cdot)$ with geometric multiplicity $geo_T(\lambda) = J$. This means that there are exactly J right and J left Jordan chains associated with λ, namely

$$\begin{aligned}(4.1)\qquad &\{\varphi_{1,0}, \ldots, \varphi_{1,m_1-1}\}, \{\varphi_{2,0}, \ldots, \varphi_{2,m_2-1}\}, \ldots, \{\varphi_{J,0}, \ldots, \varphi_{J,m_J-1}\}, \quad \text{and}\\ &\{\psi_{1,0}, \ldots, \psi_{1,m_1-1}\}, \{\psi_{2,0}, \ldots, \psi_{2,m_2-1}\}, \ldots, \{\psi_{J,0}, \ldots, \psi_{J,m_J-1}\},\end{aligned}$$

where $m_i \geq 2$ $(1 \leq i \leq J)$, such that they satisfy the properties described in Theorem 2.3. Consider a singular value decomposition of $T(\lambda)$ in the following form

$$Y^*T(\lambda)X = \begin{bmatrix} 0_J & 0 \\ 0 & \Sigma_{n-J} \end{bmatrix},$$

where $X = [X_J \ X_{n-J}]$ and $Y = [Y_J \ Y_{n-J}]$ are unitary matrices, $X_J \in \mathbb{C}^{n\times J}$ and $Y_J \in \mathbb{C}^{n\times J}$ have orthonormal columns forming a basis of $\text{span}\{\varphi_{1,0}, \ldots, \varphi_{J,0}\}$ and $\text{span}\{\psi_{1,0}, \ldots, \psi_{J,0}\}$, respectively, and Σ_{n-J} is a diagonal matrix of nonzero singular values of $T(\lambda)$. Therefore, there exist nonsingular matrices $K_J, M_J \in \mathbb{C}^{J\times J}$ such that $X_J = [\varphi_{1,0} \ \ldots \ \varphi_{J,0}]K_J$ and $Y_J = [\psi_{1,0} \ \ldots \ \psi_{J,0}]M_J$. Let $v = [\varphi_{1,0} \ \ldots \ \varphi_{J,0}]d_v$ be a candidate right eigenvector where $d_v \neq 0$. It follows from (2.11) that

$$Y_J^*T'(\lambda)v = M_J^*[\psi_1 \ \ldots \ \psi_J]^*T'(\lambda)[\varphi_1 \ \ldots \ \varphi_J]d_v = 0.$$

Thus we have

$$\begin{bmatrix} Y^* & \\ & 1 \end{bmatrix} \begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix} \begin{bmatrix} X & \\ & 1 \end{bmatrix} = \begin{bmatrix} Y^*T(\lambda)X & Y^*T'(\lambda)v \\ u^*X & 0 \end{bmatrix}$$
$$= \begin{bmatrix} 0_J & 0 & 0 \\ 0 & \Sigma_{n-J} & Y_{n-J}^*T'(\lambda)v \\ u^*X_J & u^*X_{n-J} & 0 \end{bmatrix}.$$

Let $h = [h_a^* \ h_b^* \ \bar{h}_c]^*$ be a vector in the null space of the above square matrix, where $h_a \in \mathbb{C}^J$, $h_b \in \mathbb{C}^{n-J}$ and $h_c \in \mathbb{C}$. Then

$$\begin{bmatrix} 0_J & 0 & 0 \\ 0 & \Sigma_{n-J} & Y_{n-J}^*T'(\lambda)v \\ u^*X_J & u^*X_{n-J} & 0 \end{bmatrix} \begin{bmatrix} h_a \\ h_b \\ h_c \end{bmatrix} = \begin{bmatrix} 0 \\ \Sigma_{n-J}h_b + Y_{n-J}^*T'(\lambda)vh_c \\ u^*X_Jh_a + u^*X_{n-J}h_b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

It follows from the second block row that $h_b = -\Sigma_{n-J}^{-1}Y_{n-J}^*T'(\lambda)vh_c$, and thus the last row is equivalent to $u^*X_Jh_a - u^*X_{n-J}\Sigma_{n-J}^{-1}Y_{n-J}^*T'(\lambda)vh_c = 0$. Since u specifies the scaling of $v = [\varphi_{1,0} \ \ldots \ \varphi_{J,0}]d_v \in \text{range}(X_J)$ such that $u^*v = 1$, we have $u^*X_J \neq 0$. Without loss of generality, assume that $u^*X_J = [\gamma_1 \ \ldots \ \gamma_J]$ where $\gamma_J \neq 0$. Then, depending on whether $h_c = 0$, we can determine h_a, h_b and h as follows

$$h = \begin{bmatrix} h_a \\ h_b \\ h_c \end{bmatrix} \in \text{span}\left\{ \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ -\frac{\gamma_1}{\gamma_J} \\ 0_{n-J} \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ -\frac{\gamma_{J-1}}{\gamma_J} \\ 0_{n-J} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \eta \\ w \\ 1 \end{bmatrix} \right\}.$$

where $\eta = \frac{1}{\gamma_J}u^*X_{n-J}\Sigma_{n-J}^{-1}Y_{n-J}^*T'(\lambda)v \in \mathbb{C}$ and $w = -\Sigma_{n-J}^{-1}Y_{n-J}^*T'(\lambda)v \in \mathbb{C}^{n-J}$. It follows that the null space $\mathcal{N}_1$ of the Jacobian at (λ, v) is of dimension J, which is

one dimension larger than that in the semi-simple case; see (3.2). In fact,

$$\mathcal{N}_1 \equiv \text{null}\left(\begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix}\right) \tag{4.2}$$

$$= \begin{bmatrix} X & \\ & 1 \end{bmatrix} \text{span}\left\{\begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ -\frac{\gamma_1}{\gamma_J} \\ 0_{n-J} \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ -\frac{\gamma_{J-1}}{\gamma_J} \\ 0_{n-J} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \eta \\ w \\ 1 \end{bmatrix}\right\}$$

$$= \text{span}\left\{\begin{bmatrix} Xe_1 - \frac{\gamma_1}{\gamma_J} Xe_J \\ 0 \end{bmatrix}, \ldots, \begin{bmatrix} Xe_{J-1} - \frac{\gamma_{J-1}}{\gamma_J} Xe_J \\ 0 \end{bmatrix}\right\}$$

$$\oplus \text{span}\left\{\begin{bmatrix} \eta Xe_J + X_{n-J} w \\ 1 \end{bmatrix}\right\}.$$

The complementary space $\mathcal{M}_1$ of $\mathcal{N}_1$ can be defined as follows

$$\mathcal{M}_1 = \text{span}\left\{\begin{bmatrix} Xe_J \\ 0 \end{bmatrix}\right\} \oplus \text{range}\left(\begin{bmatrix} X_{n-J} \\ 0 \end{bmatrix}\right), \tag{4.3}$$

so that $\dim(\mathcal{M}_1) = n-J+1$, and $\mathbb{C}^{n+1} = \mathcal{N}_1 \oplus \mathcal{M}_1$. From (4.2) and (4.3), it follows by the definitions of $\mathcal{N}_1$ and $\mathcal{M}_1$ that

$$\mathcal{M}_2 = \text{range}\left(\begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix}\right) = \begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u^* & 0 \end{bmatrix} \mathcal{M}_1 \tag{4.4}$$

$$= \text{span}\left\{\begin{bmatrix} 0 \\ 1 \end{bmatrix}\right\} \oplus \text{range}\left(\begin{bmatrix} T(\lambda)X_{n-J} \\ u^* X_{n-J} \end{bmatrix}\right), \ (u^* X e_J = \gamma_J \neq 0 \text{ by assumption})$$

so that $\dim(\mathcal{M}_2) = n - J + 1$. There is considerable freedom to choose the complementary space $\mathcal{N}_2$; for example, one can define

$$\mathcal{N}_2 = \text{range}\left(\begin{bmatrix} \big(T(\lambda)X_{n-J}\big)^{\perp} \\ 0 \end{bmatrix}\right), \tag{4.5}$$

where $\big(T(\lambda)X_{n-J}\big)^{\perp}$ consists of J column vectors orthogonal to range$\big(T(\lambda)X_{n-J}\big)$, and therefore $\mathcal{M}2$ and $\mathcal{N}_2$ are orthogonal complements of each other.

Similar to the analysis for semi-simple eigenvalues, let $e_k = \begin{bmatrix} x_k \\ \mu_k \end{bmatrix} - \begin{bmatrix} v \\ \lambda \end{bmatrix}$ be the error between the Newton iterate and the *particular eigenpair* (λ, v) in the kth step, $\mathcal{P}_{\mathcal{N}_1}$ be the projector onto $\mathcal{N}_1$ along $\mathcal{M}_1$, and $\mathcal{P}_{\mathcal{M}_1} = I - \mathcal{P}_{\mathcal{N}_1}$. To complete the analysis, we make the following assumption.

Assumption 4.1. *For any sequence of Newton iterate errors $\{e_k\}$ whose components lying in $\mathcal{N}_1$ converge to zero linearly, their components lying in any one-dimensional subspace of $\mathcal{N}_1$ also converge to zero linearly.*

The assumption states that the Newton iterate errors lying in any subspace of the kernel of the singular Jacobian exhibit qualitatively the same behavior, and no "special" subspace exists in which the iterate errors converge more quickly than they

do in other subspaces. This assumption of isotropism is based on the observations of the behavior of Newton iterate errors in our numerical experiments.

Since the Jacobian is singular at (λ, v), Theorem 2.5 shows that $\|\mathcal{P}_{\mathcal{N}_1}(e_k)\|$ and $\|\mathcal{P}_{\mathcal{M}_1}(e_k)\|$, respectively, converge to zero linearly and quadratically. From (4.2), since $\text{span}\left\{\begin{bmatrix} \eta X e_J + X_{n-J} w \\ 1 \end{bmatrix}\right\}$ is a subspace of $\mathcal{N}_1$, by Assumption 4.1, the iterate errors $\{e_k\}$ have a component lying in this one-dimensional space which converges linearly. Given the form of this basis vector, we see that its last entry 1 represents the eigenvalue approximation error, and it also contains the component $X_{n-J}w$ which represents an eigenvector approximation error (range(X_J) is the desired eigenspace). As a result, inverse iteration converges towards λ and its eigenspace linearly.

4.2. Numerical experiments for inverse iteration. Numerical results are provided in this section to illustrate the linear convergence of inverse iteration for defective eigenvalues. We choose two problems from the NLEVP collection, and we constructed four problems artificially, because the benchmark problems in the literature with defective eigenvalues are rather limited.

A description of these problems is given in Table 4.1. For example, the problem *df_art_m1m2*, which defines an matrix pencil $T(\mu) \in \mathbb{C}^{256\times 256}$, is an artificially constructed, truly nonlinear problem. It has a defective eigenvalue $\lambda = 0$, and the algebraic and the geometric multiplicities of λ are $alg_T(\lambda) = 5$ and $geo_T(\lambda) = 4$, respectively; the length of the shortest and the longest Jordan chains associated with λ are $\min\{m_i\} = 1$ and $\max\{m_i\} = 2$, respectively.

problem	source	type	size	eigenvalue	$alg_T(\lambda)$ & $geo_T(\lambda)$	$\min\{m_i\}$ & $\max\{m_i\}$
time_delay	NLEVP	nep	3	$3\pi i$	2 1	2 2
jordan3	artificial	lep	256	2	3 1	3 3
df_art_m1m2	artificial	nep	256	0	5 4	1 2
df_art_m1m3	artificial	nep	256	0	5 3	1 3
df_art_m2m3	artificial	nep	256	0	5 2	2 3
mirror	NLEVP	pep	9	0	9 7	1 2

TABLE 4.1
Description of the test problems for defective eigenvalues

The four artificially constructed problems are as follows. For *jordan3*,

$$T(\mu) = G_A^* D(\mu) G_B, \qquad \text{where}$$
$$D(\mu) = \begin{bmatrix} \mu-2 & -1 & & \\ & \mu-2 & -1 & \\ & & \mu-2 & \\ & & & \mu I_{253} - diag([0;\, 1;\, c_1]) \end{bmatrix},$$

and for the other three problems,

$$T(\mu) = G_A^* \begin{bmatrix} D_5(\mu) & \\ & diag([c_0 + \mu c_1 + \mu^2 c_2]) \end{bmatrix} G_B, \qquad \text{where}$$
$$D_5(\mu) = \begin{bmatrix} e^{\mu}-1 & 1-\tan^{-1}(2\mu) & & & & \\ & 2\sin(\mu) & & & & \\ & & -5\ln(1+\mu) & & & \\ & & & 8\mu & & \\ & & & & \tan^{-1}(3\mu) & \end{bmatrix}$$

for *df_art_m*1*m*2,

$$D_5(\mu) = \begin{bmatrix} e^{\mu}-1 & 1-\tan^{-1}(2\mu) & & & & \\ & 2\sin(\mu) & \cos(\mu^2) & & & \\ & & -5\ln(1+\mu) & & & \\ & & & 8\mu & & \\ & & & & \tan^{-1}(3\mu) & \end{bmatrix}$$

for *df_art_m*1*m*3, and

$$D_5(\mu) = \begin{bmatrix} e^{\mu}-1 & 1-\tan^{-1}(2\mu) & & & & \\ & 2\sin(\mu) & \cos(\mu^2) & & & \\ & & -5\ln(1+\mu) & & & \\ & & & 8\mu & e^{-2\mu} & \\ & & & & \tan^{-1}(3\mu) & \end{bmatrix}$$

*df_art_m*2*m*3, respectively, where G_A, G_B and c_i $(i = 0, 1, 2)$ are random matrices described in Section 3.2. Among the six test problems, *time_delay*, *jordan*3 and *df_art_m*2*m*3 have Jordan chains of minimum length ≥ 2. The linear convergence of inverse iteration for this type of problem is shown in Section 4.1.

To illustrate the analysis, we generated an initial eigenpair approximation (μ_0, x_0) in the same manner as we did for semi-simple eigenvalues. We then ran inverse iteration with (μ_0, x_0), and we found that the algorithm does converge linearly until the eigenvalue and eigenvector approximation errors decrease to the magnitude around $\epsilon^{1/\max\{m_i\}}$ (ϵ is the machine precision) — the highest precision one can achieve by a single-vector algorithm for defective eigenvalues; see [19] for details. An estimate of the order of convergence was obtained by applying the least-squares line formula to the sequence $(\log e_k, \log e_{k+1})$ for $k = 1, 2, \ldots$, where $e_k := \|T(\mu_k)x_k\|$. Note that we did not use e_0, because the residual norm $\|T(\mu_1)x_1\|$ is usually significantly smaller than $\|T(\mu_0)x_0\|$ (see Lemma 4.5 for an explanation), and thus the inclusion of e_0 produces considerable noise in our estimate. Table 4.2 shows that inverse iteration converges linearly for defective eigenvalues λ for which the shortest Jordan chain is of length ≥ 2.

problem	$\angle(x_0^{(1)}, v)$	# iters	estimated ℓ
time_delay	$\times 10^{-3}$	20	1.001
*jordan*3	5×10^{-3}	14	0.984
*df_art_m*2*m*3	10^{-2}	15	0.969

TABLE 4.2
Estimated order of convergence of inverse iteration for a defective λ $(\min\{m_i\} \geq 2)$

4.3. Rayleigh functional iteration and single-vector JD. The linear convergence of inverse iteration towards defective eigenpairs is much less satisfactory than its quadratic convergence towards semi-simple eigenpairs. Thus it is important to develop algorithms that converge more rapidly. By analogy with the order of convergence exhibited by the Newton-like methods for semi-simple eigenvalues, one might speculate that RFI and single-vector JD exhibit quadratic convergence towards defective eigenpairs for locally symmetric problems. Unfortunately, this is not the case, as we show later in Proposition 4.2, due to the special structure of the resolvent near defective eigenvalues. In fact, RFI generally converges only linearly towards defective eigenpairs, whether the local symmetry of $T(\cdot)$ exists or not.

To see this, we first assume for the sake of simplicity that the defective λ has only one right Jordan chain $\{\varphi_{1,0},\ldots,\varphi_{1,m-1}\}$ such that $alg_T(\lambda)=m$ and $geo_T(\lambda)=1$. Let (μ,x) be an eigenpair approximation, and $p=T^{-1}(\mu)T'(\mu)x$ be the unnormalized new eigenvector approximation computed by any Newton-like method we discussed. Recalling the structure of $T^{-1}(\mu)$ from Theorem 2.3, we have

$$
\begin{aligned}
(4.6)\qquad p=T^{-1}(\mu)T'(\mu)x &= \sum_{h=0}^{m-1}\frac{\sum_{s=0}^{h}\langle T'(\mu)x,\psi_{1,s}\rangle\varphi_{1,h-s}}{(\mu-\lambda)^{m-h}}+Q(\mu)T'(\mu)x\\
&=\sum_{i=0}^{m-1}\frac{\langle T'(\mu)x,\psi_{1,0}\rangle}{(\mu-\lambda)^{m-i}}\varphi_{1,i}+\sum_{i=0}^{m-2}\frac{\langle T'(\mu)x,\psi_{1,1}\rangle}{(\mu-\lambda)^{m-1-i}}\varphi_{1,i}+\cdots\\
&\qquad+\sum_{i=0}^{1}\frac{\langle T'(\mu)x,\psi_{1,m-2}\rangle}{(\mu-\lambda)^{2-i}}\varphi_{1,i}+\frac{\langle T'(\mu)x,\psi_{1,m-1}\rangle}{(\mu-\lambda)}\varphi_{1,0}+Q(\mu)T'(\mu)x\\
&=\sum_{j=0}^{m-1}\sum_{i=0}^{m-j-1}\frac{\langle T'(\mu)x,\psi_{1,j}\rangle}{(\mu-\lambda)^{m-j-i}}\varphi_{1,i}+Q(\mu)T'(\mu)x.
\end{aligned}
$$

To analyze the direction of p, assume that the eigenvector $\varphi_{1,0}$ and the generalized eigenvector $\varphi_{1,1}$ are not parallel. Then for every $j<m-1$, consider the following component shown in the last equation of (4.6)

$$
(4.7)\qquad \sum_{i=0}^{m-j-1}\frac{\langle T'(\mu)x,\psi_{1,j}\rangle}{(\mu-\lambda)^{m-j-i}}\varphi_{1,i}=\frac{\langle T'(\mu)x,\psi_{1,j}\rangle}{(\mu-\lambda)^{m-j}}\sum_{i=0}^{m-j-1}(\mu-\lambda)^i\varphi_{1,i}.
$$

The above expression shows clearly that the ratio between the magnitude of the error component (in the direction of $\varphi_{1,1}$) and the magnitude of the eigenvector component (in the direction of $\varphi_{1,0}$) in (4.7) is on the order of $\mathcal{O}(\mu-\lambda)$. Now for $j=m-1$ in (4.6), assume in addition that $\langle T'(\lambda)\varphi_{1,0},\psi_{1,m-1}\rangle\neq 0$, so that $\langle T'(\mu)x,\psi_{1,m-1}\rangle\approx\langle T'(\lambda)\varphi_{1,0},\psi_{1,m-1}\rangle=\mathcal{O}(1)$ for μ sufficiently close to λ and x sufficiently close to $\varphi_{1,0}$ in direction. Consider the corresponding component in the last equation of (4.6), namely,

$$
(4.8)\qquad \frac{\langle T'(\mu)x,\psi_{1,m-1}\rangle}{\mu-\lambda}\varphi_{1,0}+Q(\mu)T'(\mu)x.
$$

Similarly, the ratio between the magnitude of the error component and that of the eigenvector component of (4.8) is also on the order of $\mathcal{O}(\mu-\lambda)$. Therefore, when normalized, the new eigenvector approximation p in (4.6) has an eigenvector component of magnitude $\mathcal{O}(1)$ and an error component of magnitude $\mathcal{O}(\mu-\lambda)$.

As a result, the local convergence rates of Newton-like methods depend on the accuracy of the eigenvalue approximation μ, which in turn usually depends on the accuracy of the eigenvector approximation x. Let the accuracy of x be represented by the sine of the error angle $\angle(x,\varphi_{1,0})$, and assume that $|\mu-\lambda|=\mathcal{O}(\sin^{\ell}\angle(x,\varphi_{1,0}))$. Then the convergence of the Newton-like method is of order ℓ. In particular, for RFI where $\mu=\rho_F(x;T,y)$ is the Rayleigh functional value, we have $\ell=1$ in general for defective eigenvalues, and therefore RFI converges only linearly. This observation is summarized as follows.

PROPOSITION 4.2. *Let λ be a defective eigenvalue of the holomorphic operator $T(\cdot):U\to\mathbb{C}^{n\times n}$, and φ and ψ be a corresponding unit right and a unit left eigenvector, respectively. Let $x=\varphi\cos\alpha+\varphi_{\perp}\sin\alpha$ and $y=\psi\cos\beta+\psi_{\perp}\sin\beta$, where $\alpha,\beta<\frac{\pi}{2}$,*

$\varphi_\perp \perp \mathrm{null}\,(T(\lambda))$ and $\psi_\perp \perp \mathrm{null}\,((T(\lambda))^*)$ are unit vectors, and thus $\|x\| = \|y\| = 1$. Assume that $y^*T'(\lambda)x \neq 0$. Let $\rho = \rho_F(x;T,y)$ be the Rayleigh functional value closest to λ such that $y^*T(\rho)x = 0$. Then for sufficiently small α,

$$|\rho - \lambda| \leq \frac{2\|T(\lambda)\|\,|\sin\alpha \sin\beta|}{|y^*T'(\lambda)x|} \tag{4.9}$$
$$= \frac{2\|T(\lambda)\|\,|\sin\alpha \sin\beta|}{\left|\overline{\cos\beta}\sin\alpha\psi^*T'(\lambda)\varphi_\perp + \overline{\sin\beta}\cos\alpha\psi_\perp^*T'(\lambda)\varphi + \overline{\sin\beta}\sin\alpha\psi_\perp^*T'(\lambda)\varphi_\perp\right|}\,.$$

Assume in addition that $\psi^*T'(\lambda)\varphi_\perp$, $\psi_\perp^*T'(\lambda)\varphi$ and $\psi_\perp^*T'(\lambda)\varphi_\perp$ are all bounded away from zero. Then, for sufficiently small α, $|\rho - \lambda| \leq \mathcal{O}(\sin\alpha)$.

Proof. The first part of the proposition through (4.9) was shown in [29, Section 4.3] using the Newton-Kantorovich Theorem. The goal here is to show that, in contrast to the scenario for semi-simple eigenvalues, we have $|\rho - \lambda| \leq \mathcal{O}(\sin\alpha)$ (instead of $\mathcal{O}(\sin\alpha\sin\beta)$), whether the local symmetry of $T(\cdot)$ exists or not.

First, assume that y is not a good left eigenvector approximation, i.e., $\sin\beta = \mathcal{O}(1)$. Since $\sin\alpha$ is small, we have $2\|T(\lambda)\|\,|\sin\alpha\sin\beta| = \mathcal{O}(\sin\alpha)$, and from (4.9), $|y^*T'(\lambda)x| = |\overline{\sin\beta}\cos\alpha\psi_\perp^*T'(\lambda)\varphi + \mathcal{O}(\sin\alpha)| = \mathcal{O}(1)$. Therefore it follows that

$$|\rho - \lambda| \leq \frac{2\|T(\lambda)\|\,|\sin\alpha\sin\beta|}{|y^*T(\lambda)x|} = \mathcal{O}(\sin\alpha). \tag{4.10}$$

Now assume that y is a good left eigenvector approximation such that $\sin\beta = \mathcal{O}(\sin\alpha)$; in particular, suppose the local symmetry of $T(\cdot)$ exists, and thus we choose $y = x$ or $y = \bar{x}$ to generate the two-sided Rayleigh functional value. In this case, $|\sin\alpha| = |\sin\beta|$, and it follows from (4.9) that $2\|T(\lambda)\|\,|\sin\alpha\sin\beta| = \mathcal{O}(\sin^2\alpha)$, and $|y^*T'(\lambda)x| = \mathcal{O}(\sin\alpha)$. Therefore, (4.10) still holds. ∎

Remark. Proposition 4.2 shows that for a defective λ, the use of a left eigenvector approximation for the Rayleigh functional ρ_F does not generate an eigenvalue approximation of second order accuracy, as is achieved for simple and semi-simple eigenvalues. This lack of high accuracy is attributed to the fact that $\psi^*T'(\lambda)\varphi = 0$. Moreover, the use of a left eigenvector approximation for ρ_F could introduce additional complications. Namely, since $|y^*T'(\lambda)x| = \mathcal{O}(\sin\alpha)$ from (4.9), it follows that $|y^*T'(\rho)x| \leq |y^*T'(\lambda)x| + \mathcal{O}(\rho - \lambda) = \mathcal{O}(\sin\alpha)$. Thus there is a risk that $y^*T'(\rho)x \neq 0$, a critical condition required by the definition of Rayleigh functionals (see [26]), may be violated, at least numerically. As a result, we see from (2.16) that the small magnitude of $y^*T'(\rho)x$ could introduce numerical difficulties in the projector $\Pi_k^{(1)}$ for single-vector JD. We therefore recommend using y far from a left eigenvector approximation to compute the Rayleigh functional value for a defective λ.

From Proposition 4.2, it follows immediately from (4.7) and (4.8) that RFI converges linearly towards defective eigenvalues. In addition, assuming that the Rayleigh functional value $\rho = \rho_F(x;T,y)$ satisfies $\langle T'(\rho)x, y\rangle \neq 0$, then the single-vector JD (2.16) also converges linearly in this case, because it is mathematically equivalent to RFI. We summarize this result in the following theorem.

THEOREM 4.3. *Let λ be a defective eigenvalue of the holomorphic operator $T(\cdot) : U \to \mathbb{C}^{n\times n}$ with exactly one left and one right Jordan chains $\{\varphi_{1,0},\ldots,\varphi_{1,m-1}\}$ and $\{\psi_{1,0},\ldots,\psi_{1,m-1}\}$, where $\varphi_{1,0}$ is not parallel to $\varphi_{1,1}$, and $\langle T'(\lambda)\varphi_{1,0}, \psi_{1,m-1}\rangle \neq 0$. Let (ρ_0, x_0) be an initial eigenpair approximation with $\angle(x_0,\varphi_{1,0})$ sufficiently small, and $\rho_k = \rho_F(x_k;T,y_k)$ be the Rayleigh functional value closest to λ. Assume that the upper bounds in* Proposition 4.2 *are qualitatively sharp, i.e., $|\rho_k - \lambda| = \mathcal{O}(\sin\angle(x_k,\varphi_{1,0}))$.*

Then RFI converges locally towards $(\lambda, \varphi_{1,0})$ *linearly. The same conclusion applies to single-vector JD* (2.16) *if, in addition,* ρ_k *is such that* $y_k^* T'(\rho_k) x_k \neq 0$.

4.4. Numerical experiments for RFI/JD. In this section, we illustrate by numerical experiments the linear convergence of RFI and single-vector JD for defective eigenvalues with a single Jordan chain. The experiments are performed on the problems *time_delay* and *jordan*3. We run RFI with an initial eigenpair approximation (μ_0, x_0), and we analyze $(\log e_k, \log e_{k+1})$, where $e_k := \|T(\mu_k)x_k\|$ $(k = 1, 2, \ldots)$, for the estimated order of convergence. Here, note that the local symmetry does not exist for both test problems, and we choose $y = T'(\lambda)x_k$ to generate the value of the Rayleigh functional $\rho_F(x_k; T, y)$. Table 4.3 shows the error angle of the initial iterate, the number of iterations taken, and the estimated order of convergence. We see clearly that RFI converges linearly for both problems.

In addition, we tested the convergence of the two-sided Rayleigh functiona iteration (TSRFI), which converges cubically for simple eigenvalues; see, e.g., [25]. We found that this algorithm also converges linearly in this setting, which is consistent with Proposition 4.2 and Theorem 4.3. As we have discussed, for a defective eigenvalue λ with a single Jordan chain, we generally have $|\rho_F(x; T, y) - \lambda| = \mathcal{O}\big(\angle(x, v)\big)$ (instead of $\mathcal{O}\big(\angle(x, v)^2\big)$), no matter whether y is a good left eigenvector approximation; consequently, TSRFI exhibits the same order of convergence (linear) as RFI. The results for TSRFI are also summarized in Table 4.3.

		RFI		TSRFI	
problem	$\angle(x_0, v)$	# iters	estimated ℓ	# iters	estimated ℓ
time_delay	10^{-3}	18	1.002	15	0.981
*jordan*3	5×10^{-3}	19	0.961	13	0.967

TABLE 4.3
Estimated order of convergence of RFI and TSRFI for a defective λ $(geo_T(\lambda) = 1)$

4.5. Accelerated algorithms. In this section, we first study an accelerated inverse iteration for degenerate eigenvalues, which is inspired by the accelerated Newton's method for general nonlinear system of equations near singular roots [8]. This algorithm, which requires the solution of two linear systems in each iteration, exhibits quadratic convergence towards defective eigenpairs. We then propose an accelerated single-vector Jacobi-Davidson method based on a minor modification of the accelerated inverse iteration, and we show by experiments that it also converges quadratically.

4.5.1. Accelerated inverse iteration. Let λ be a defective eigenvalue of the holomorphic $T(\cdot)$. To simplify the notation, we use the MATLAB expressions to denote eigenpair approximations written in the form of column vectors; e.g., $[x; \mu]$ is used to represent $\begin{bmatrix} x \\ \mu \end{bmatrix}$. Let $F([v; \lambda]) = 0$ be the augmented system of (1.1), and $[x_k; \mu_k]$ be the starting eigenpair approximation in the kth iteration. Consider the following accelerated Newton's method:

$$
\begin{aligned}
[w_k; \nu_k] &= [x_k; \mu_k] - F'([x_k; \mu_k])^{-1} F([x_k; \mu_k]) \qquad \text{(half-step iterate)} \\
[x_{k+1};\, \mu_{k+1}] &= [w_k; \nu_k] - m F'([w_k; \nu_k])^{-1} F([w_k; \nu_k]) \qquad \text{(full-step iterate)} \\
&= m\left([w_k; \nu_k] - F'([w_k; \nu_k])^{-1} F([w_k; \nu_k])\right) - (m-1)[w_k; \nu_k],
\end{aligned} \tag{4.11}
$$

where $F([x_k;\mu_k]) = \begin{bmatrix} T(\mu_k)x_k \\ u^*x_k - 1 \end{bmatrix} = \begin{bmatrix} T(\mu_k)x_k \\ 0 \end{bmatrix}$, $\|F([x_k;\mu_k])\| = \|T(\mu_k)x_k\|$ is the residual norm of $[x_k;\mu_k]$, and $F'([x_k;\mu_k]) = \begin{bmatrix} T(\mu_k) & T'(\mu_k)x_k \\ u^* & 0 \end{bmatrix}$ is the Jacobian of F at $[x_k;\mu_k]$. In other words, the full-step eigenpair approximation $[x_{k+1};\mu_{k+1}]$ is a special linear combination of the half-step iterate $[w_k;\nu_k]$ and the next standard Newton's iterate $[w_k;\nu_k] - F'([w_k;\nu_k])^{-1}F([w_k;\nu_k])$. We will see later in this section that the length of the Jordan chain m is the only value for the linear combination coefficients in (4.11) such that the algorithm converges quadratically.

It can be shown by the structure of the block inverse of the Jacobian that (4.11) is equivalent to the following accelerated inverse iteration:

$$
(4.12)\quad \begin{cases}
1.\ p_k = T^{-1}(\mu_k)T'(\mu_k)x_k & \text{(half-step intermediate vector)} \\
2.\ w_k = \dfrac{p_k}{u^*p_k} & \text{(half-step eigenvector approximation)} \\
3.\ \nu_k = \mu_k - \dfrac{1}{u^*p_k} & \text{(half-step eigenvalue approximation)} \\
4.\ q_k = T^{-1}(\nu_k)T'(\nu_k)w_k & \text{(full-step intermediate vector)} \\
5.\ x_{k+1} = -(m-1)w_k + m\dfrac{q_k}{u^*q_k} & \text{(full-step eigenvector approximation)} \\
6.\ \mu_{k+1} = \nu_k - \dfrac{m}{u^*q_k} & \text{(full-step eigenvalue approximation)}
\end{cases}.
$$

In this section, we establish the locally quadratic convergence of the accelerated algorithm (4.11) (or (4.12)) towards the desired defective eigenpair. To this end, we first make an assumption about the eigenpair approximation (μ_k, x_k) as follows.

ASSUMPTION 4.4. *Let λ be a defective eigenvalue of the holomorphic $T(\cdot)$ with J right and J left Jordan chains shown in* (4.1)*. Assume that the eigenpair approximation (μ_k, x_k) is such that its eigenvalue approximation error $|\mu_k - \lambda|$ is proportional to its eigenvector approximation error $\angle(x_k, \Phi)$ where $\Phi = \operatorname{span}\{\varphi_{1,0}, \ldots, \varphi_{J,0}\}$.*

This assumption seems reasonable due to the following observation. In practice, it is usually not known in priori whether the desired eigenpair is defective, and thus we use Newton's method, RFI or JD to solve for the eigenpair. For Newton's method, it is shown in Section 4.1 that its local convergence towards a defective eigenpair is linear; in fact, the error $e_k = [x_k;\mu_k] - [v;\lambda]$ has a component in the one-dimensional space $\operatorname{span}\left\{\begin{bmatrix} \eta X e_J + X_{n-J}w \\ 1 \end{bmatrix}\right\}$ (a subspace of the null space of the Jacobian) which converges linearly. Since this basis vector has nontrivial components representing both eigenvalue and eigenvector approximation errors, the two errors become proportional to each other after sufficiently many Newton steps. This assumption also holds for RFI where $\mu_k = \rho$ is the Rayleigh functional value, since Proposition 4.2 shows that $|\rho - \lambda| \le \mathcal{O}(\sin\angle(x_k, \Phi))$ for the defective λ, independent of the symmetry of $T(\lambda)$.

Our main goal is to show that the accelerated method (4.11) converges quadratically towards the defective eigenpair $[v;\lambda]$. We take three steps to complete this analysis. In step 1, we make a few assumptions about the half-step iterate $[w_k;\nu_k]$, and we study the values of b, c, d in the Taylor expansion of $F([w_k;\nu_k])$ at $[v;\lambda]$. This step is critical to establish the quadratic convergence. In step 2, we show that the Jacobian at any eigenpair approximation sufficiently close to $[v;\lambda]$ is nonsingular, so that all half-step and full-step iterates are well-defined. In step 3, we write the full-step iterate error as a linear combination of the error of $[w_k;\nu_k]$ and that of the next standard Newton iterate $[z_k;\xi_k] = [w_k;\nu_k] - F'([w_k;\nu_k])^{-1}F([w_k;\nu_k])$; we analyze

the projections of the full-step iterate error onto $\mathcal{M}_1$ and $\mathcal{N}_1$, and show that all the projected errors are bounded by $\mathcal{O}(s_k^2)$, where $s_k = \sin\angle(x_k, \varphi_{1,0})$, the error angle between the current eigenvector approximation and the desired eigenvector.

In the following analysis, to simplify the notation, we omit the subscript k of s_k, c_k, $[x_k;\mu_k]$, and $[w_k;\nu_k]$, when there is no risk of confusion; we keep the subscript $k+1$ of $[x_{k+1};\mu_{k+1}]$ though, to clearly identify the full-step iterate. To simplify the analysis, we again assume that λ has only one right Jordan chain $\{\varphi_{1,0},\ldots,\varphi_{1,m-1}\}$.

In step 1, we first show that the half-step iterate $[w;\nu]$ has a special property as follows. Since Newton's method converges linearly, the error of $[w;\nu]$ is proportional to that of $[x;\mu]$, yet the residual norm of $[w;\nu]$ is significantly smaller than that of $[x;\mu]$; namely, $\|T(\mu)x\| = \mathcal{O}(s)$ and $\|T(\nu)w\| = \mathcal{O}(s^m)$, where $s = \sin\angle(x,\varphi_{1,0})$ is the eigenvector approximation error.

LEMMA 4.5. *Let λ be a defective eigenvalue of the holomorphic operator $T(\cdot)$ with only one left and one right Jordan chains $\{\varphi_{1,0},\ldots,\varphi_{1,m-1}\}$ and $\{\psi_{1,0},\ldots,\psi_{1,m-1}\}$. Assume that $\langle T''(\lambda)\varphi_{1,0},\psi_{1,0}\rangle \neq 0$, or $\langle T'(\lambda)\varphi_{1,0},\psi_{1,1}\rangle \neq 0$. Let $[x;\mu]$ be an eigenpair approximation satisfying Assumption 4.4, $s = \sin\angle(x,\varphi_{1,0})$ be the sine of the error angle of x, and $[w;\nu]$ be the half-step iterate in (4.11). Then $\|T(\nu)w\| = \mathcal{O}(s^m)$ for sufficiently small s.*

Proof. We first establish two critical relations, namely, $\|u^*T^{-1}(\mu)T'(\mu)x\| = \mathcal{O}(s^{-(m-1)})$ and $\|T'(\mu)x - T'(\mu)w\| = \mathcal{O}(s)$. Assume without loss of generality that $x = c\varphi_{1,0} + sg$, where $\|\varphi_{1,0}\| = \|g\| = 1$ and $g \perp \varphi_{1,0}$.

We first show that $\|u^*T^{-1}(\mu)T'(\mu)x\| = \mathcal{O}(s^{-(m-1)})$. From (4.6), we have that

$$p = T^{-1}(\mu)T'(\mu)x = \sum_{j=0}^{m-1}\sum_{i=0}^{m-j-1}\frac{\langle T'(\mu)x,\psi_{1,j}\rangle}{(\mu-\lambda)^{m-j-i}}\varphi_{1,i} + G(\mu)T'(\mu)x \tag{4.13}$$
$$= \sum_{i=0}^{m-1}\frac{\langle T'(\mu)x,\psi_{1,0}\rangle}{(\mu-\lambda)^{m-i}}\varphi_{1,i} + \sum_{j=1}^{m-1}\sum_{i=0}^{m-j-1}\frac{\langle T'(\mu)x,\psi_{1,j}\rangle}{(\mu-\lambda)^{m-j-i}}\varphi_{1,i} + G(\mu)T'(\mu)x.$$

Recall from (2.11) that $\langle T'(\lambda)\varphi_{1,0},\psi_{1,0}\rangle = 0$, and $|\mu-\lambda| = \mathcal{O}(s)$ by Assumption 4.4. First, assume that $\langle T''(\lambda)\varphi_{1,0},\psi_{1,0}\rangle = \mathcal{O}(1)$. Then

$$\begin{aligned}\langle T'(\mu)x,\psi_{1,0}\rangle &= c\langle T'(\mu)\varphi_{1,0},\psi_{1,0}\rangle + s\langle T'(\mu)g,\psi_{1,0}\rangle \\ &= c\langle T'(\lambda)\varphi_{1,0},\psi_{1,0}\rangle + c(\mu-\lambda)\langle T''(\lambda)\varphi_{1,0},\psi_{1,0}\rangle + s\langle T'(\lambda)g,\psi_{1,0}\rangle \\ &\quad + \mathcal{O}\left((\mu-\lambda)^2\right) + \mathcal{O}\left(s(\mu-\lambda)\right) \\ &= 0 + \mathcal{O}(\mu-\lambda) + \mathcal{O}(s) = \mathcal{O}(s).\end{aligned} \tag{4.14}$$

The dominant term in $\sum_{i=0}^{m-1}\langle T'(\mu)x,\psi_{1,0}\rangle(\mu-\lambda)^{-(m-i)}\varphi_{1,i}$, which appears in the last equality of (4.13), is thus

$$\frac{\langle T'(\mu)x,\psi_{1,0}\rangle}{(\mu-\lambda)^m}\varphi_{1,0} = \frac{\mathcal{O}(s)}{\mathcal{O}(s^m)}\varphi_{1,0} = \mathcal{O}(s^{-(m-1)})\varphi_{1,0}.$$

Consider the sum of the terms corresponding to $j=1$ in (4.13), namely,

$$\sum_{i=0}^{m-2}\frac{\langle T'(\mu)x,\psi_{1,1}\rangle}{(\mu-\lambda)^{m-1-i}}\varphi_{1,i}. \tag{4.15}$$

Now, assume alternatively that $\langle T'(\lambda)\varphi_{1,0},\psi_{1,1}\rangle \neq 0$. It follows that $\langle T'(\mu)x,\varphi_{1,1}\rangle = \langle T'(\lambda)\varphi_{1,0},\psi_{1,1}\rangle + \mathcal{O}(s) = \mathcal{O}(1)$ for small s. Therefore the dominant term in (4.15) is

$$\frac{\langle T'(\mu)x,\psi_{1,1}\rangle}{(\mu-\lambda)^{m-1}}\varphi_{1,0} = \frac{\mathcal{O}(1)}{\mathcal{O}(s^{m-1})}\varphi_{1,0} = \mathcal{O}(s^{-(m-1)})\varphi_{1,0}.$$

For every $j \geq 2$, the sum of corresponding terms in (4.13) are bounded by $\mathcal{O}(s^{-(m-2)})$, and they are thus not the dominant ones. In summary, if either $\langle T''(\lambda)\varphi_{1,0}, \psi_{1,0}\rangle \neq 0$ or $\langle T'(\lambda)\varphi_{1,0}, \psi_{1,1}\rangle \neq 0$, the dominant term in (4.13) can be written as $\mathcal{O}(s^{-(m-1)})\varphi_{1,0}$, and $\|u^*T^{-1}(\mu)T'(\mu)x\| = \mathcal{O}(s^{-(m-1)})$ follows.

To complete the proof, it is sufficient to show $\|T'(\mu)x - T'(\mu)w\| = \mathcal{O}(s)$. In fact, since $[w;\nu]$ is obtained by applying one step of Newton's method to $[x;\mu]$, and both the eigenvalue and the eigenvector approximation errors of Newton's iterates converge linearly in this case (see Section 4.1), we have $\|w - \varphi_{1,0}\| = \mathcal{O}(s)$. Therefore

$$\begin{aligned}\|T'(\mu)x - T'(\mu)w\| &\leq \|T'(\mu)\|\|x - w\| \\ &\leq \|T'(\mu)\|(\|x - \varphi_{1,0}\| + \|w - \varphi_{1,0}\|) = \mathcal{O}(s).\end{aligned}$$

Finally, note from (4.12) that

$$\begin{aligned}T(\nu)w &= T\left(\mu - [u^*T^{-1}(\mu)T'(\mu)x)]^{-1}\right)w \\ &= T(\mu)w - \frac{T'(\mu)w}{u^*T^{-1}(\mu)T'(\mu)x} + \mathcal{O}\left((u^*T^{-1}(\mu)T'(\mu)x)^{-2}\right) \\ &= T(\mu)\frac{T^{-1}(\mu)T'(\mu)x}{u^*T^{-1}(\mu)T'(\mu)x} - \frac{T'(\mu)w}{u^*T^{-1}(\mu)T'(\mu)x} + \mathcal{O}(s^{2(m-1)}) \\ &= \frac{T'(\mu)x - T'(\mu)w}{u^*T^{-1}(\mu)T'(\mu)x} + \mathcal{O}(s^{2(m-1)}).\end{aligned} \tag{4.16}$$

It then immediately follows that

$$\begin{aligned}\|T(\nu)w\| &= \frac{\|T'(\mu)x - T'(\mu)w\|}{|u^*T^{-1}(\mu)T'(\mu)x|} + \mathcal{O}(s^{2(m-1)}) \\ &= \frac{\mathcal{O}(s)}{\mathcal{O}(s^{-(m-1)})} + \mathcal{O}(s^{2(m-1)}) = \mathcal{O}(s^m)\end{aligned}$$

for $m \geq 2$. This completes the proof. □

Lemma 4.5 gives a critical preliminary result in step 1 of the proof on the values of b, c, and d in the Taylor expansion of $F([w;\nu])$ at $[\varphi_{1,0};\lambda]$. To complete this step, we need the following assumption about $[w;\nu]$.

ASSUMPTION 4.6. *Let λ be a defective eigenvalue of the holomorphic operator $T(\cdot)$ with exactly one right and one left Jordan chains. Let $\mathcal{M}_2$ defined in* (4.4) *be the range of the Jacobian at (λ, v)* (where $v = \varphi_{1,0}$)*, and $[x;\mu]$ and $[w;\nu]$ be the starting and the half-step iterates, respectively, of the accelerated method* (4.11)*. Assume that there exists a constant $\theta_0 > 0$ independent of $|\mu - \lambda|$ and $\angle(x, \varphi_{1,0})$, such that the angle between $F([w;\nu]) = \begin{bmatrix} T(\nu)w \\ 0 \end{bmatrix}$ and $\mathcal{M}_2$ is bounded below by θ_0.*

Assumption 4.6 seems reasonable in general, as we discuss below. By Lemma 4.5, $T(\nu)w$ has a significant component parallel to $T'(\mu)(w - x)$, where $w - x \perp u$ because $u^*x = u^*x = 1$. Thus $\begin{bmatrix} T(\nu)w \\ 0 \end{bmatrix}$ has a large component in $\left\{\begin{bmatrix} T'(\mu)\left(\text{span}\{u\}\right)^{\perp} \\ 0 \end{bmatrix}\right\}$, where $(\text{span}\{u\})^{\perp}$ is the orthogonal complement of $\text{span}\{u\}$. Given the structure of $\mathcal{M}_2$ in (4.4), with a proper choice of u, there is no reason to expect this component to be well approximated by any vector in $\mathcal{M}_2$.

To complete step 1, recall the Taylor expansion of $F([w;\nu])$ at $[v;\lambda]$ as follows:

$$F([w;\nu]) \equiv \begin{bmatrix} T(\nu)w \\ u^*y-1 \end{bmatrix} = \begin{bmatrix} T(\lambda)v \\ 0 \end{bmatrix} + \begin{bmatrix} T(\lambda) & T'(\lambda)v \\ u & 0 \end{bmatrix} \begin{bmatrix} y-v \\ \nu-\lambda \end{bmatrix} +$$
$$\sum_{j=1}^{n} \frac{1}{(j+1)!} \begin{bmatrix} (\nu-\lambda)^j T^{(j)}(\lambda) & \left\{ \begin{array}{c} j(\nu-\lambda)^{j-1}T^{(j)}(\lambda)(y-v) \\ +(\nu-\lambda)^j T^{(j+1)}(\lambda)v \end{array} \right\} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y-v \\ \nu-\lambda \end{bmatrix}$$
$$+\mathcal{O}(\|e_{w\nu}\|^{n+2}) = \sum_{j=0}^{n} \frac{1}{(j+1)!} F^{(j+1)}([v;\lambda])(e_{w\nu}^j, e_{w\nu}) + \mathcal{O}(\|e_{w\nu}\|^{n+2}),$$

where $e_{w\nu} = [w;\nu] - [v;\lambda]$, $F^{(j+1)}([v;\lambda])(\cdot,\cdots,\cdot) : \mathbb{C}^{n+1} \times \ldots \times \mathbb{C}^{n+1} \to \mathbb{C}^{n+1}$ stands for the $j+1$st derivative of F at $[v;\lambda]$ (which is a multilinear form (tensor) with $j+1$ arguments), and $e_{w\nu}^j$ means that the first j arguments of $F^{(j+1)}$ are all $e_{w\nu}$. In particular, $F^{(j+1)}([v;\lambda])(e_{w\nu}^j, \cdot)$ is a $\mathbb{C}^{n+1} \times \mathbb{C}^{n+1}$ matrix.

Now we are ready to discuss several cases in which the possible values of b, c, and d in the Taylor expansion of $F([w;\nu])$ at $[v;\lambda]$ can be determined.

LEMMA 4.7. *Let $[v;\lambda]$ be a defective eigenpair of $T(\cdot)$ with one right and one left Jordan chain of length m, $[x;\mu]$ a corresponding eigenpair approximation satisfying Assumption* 4.4*, and $[w;\nu]$ the half-step eigenpair approximation in* (4.11) *computed by one step of Newton's method. The Taylor expansion of $F([w;\nu])$ at $[v;\lambda]$ is*

$$F([w;\nu]) \equiv \begin{bmatrix} T(\nu)w \\ 0 \end{bmatrix} = \begin{bmatrix} T(\lambda)v \\ 0 \end{bmatrix} + A_{F^*}e_{w\nu} + \sum_{j=a}^{n} \frac{1}{j+1} A_{(j)}([w;\nu])e_{w\nu}$$
$$+ \sum_{j=b}^{n} \frac{1}{j+1} B_{(j)}([w;\nu])e_{w\nu} + \sum_{j=c}^{n} \frac{1}{j+1} C_{(j)}([w;\nu])e_{w\nu}$$
$$+ \sum_{j=d}^{n} \frac{1}{j+1} D_{(j)}([w;\nu])e_{w\nu} + \mathcal{O}(\|e_{w\nu}\|^{n+2}). \qquad (\, n \geq \max(a,b,c,d)\,)$$

Then $b = 1$ if $m > 2$. In addition, under Assumption 4.6*, exactly one the following scenarios must be true:*

1. *$c \geq d = m-1$, or*
2. *(only if $m \geq 3$) $c = m-2$ and $d \geq m-1$, or*
3. *(only if $m \geq 4$) $c \leq m-3$ and $d = c+1$.*

Proof. We know from Lemma 4.5 that $\|F([w;\nu])\| = \mathcal{O}(s^m)$. By Assumption 4.6, $\angle(F([w;\nu]), \mathcal{M}_2) > \theta_0 > 0$. From (4.4) and (4.5), since $\mathcal{M}_2$ and $\mathcal{N}_2$ are orthogonal complements, and $P_{\mathcal{N}_2}$ is the projection onto $\mathcal{N}_2$ along $\mathcal{M}_2$, we have

$$\|P_{\mathcal{N}_2}F([w;\nu])\| \geq \|F([w;\nu])\| \sin\theta_0 = \mathcal{O}(s^m) \quad \text{and}$$
$$\|P_{\mathcal{M}_2}F([w;\nu])\| \leq \|F([w;\nu])\| \cos\theta_0 = \mathcal{O}(s^\ell), \quad \text{where } \ell \geq m.$$

In addition, by Assumption 4.4, $[x;\mu]$ has eigenvalue and eigenvector approximation errors both on the order of $\mathcal{O}(s)$, and the two errors are represented by certain components lying in $\mathcal{N}_1$ and $\mathcal{M}_1$, resepectively; see (4.2) and (4.3). It follows that

$$P_{\mathcal{N}_1}e_{x\mu} = \mathcal{O}(s) \quad \text{and} \quad P_{\mathcal{M}_1}e_{x\mu} = \mathcal{O}(s), \quad \text{where } e_{x\mu} = [x;\mu] - [v;\lambda].$$

By Theorem 2.5, we have $P_{\mathcal{N}_1}e_{w\nu} = \mathcal{O}(s)$ and $P_{\mathcal{M}_1}e_{w\nu} = \mathcal{O}(s^2)$. To find the value of

b for $m > 2$, note that

$$\begin{aligned} P_{\mathcal{M}_2}F([w;\nu]) &= A_{F^*}e_{w\nu} + \sum_{j=a}^{n}\frac{1}{j+1}A_{(j)}([w;\nu])e_{w\nu} + \sum_{j=b}^{n}\frac{1}{j+1}B_{(j)}([w;\nu])e_{w\nu} \\ &= A_{F^*}(P_{\mathcal{M}_1}e_{w\nu}) + \sum_{j=a}^{n}\frac{1}{j+1}A_{(j)}([w;\nu])(P_{\mathcal{M}_1}e_{w\nu}) + \sum_{j=b}^{n}\frac{1}{j+1}B_{(j)}([w;\nu])(P_{\mathcal{N}_1}e_{w\nu}) \\ &= \mathcal{O}(s^2) + \mathcal{O}(s^{a+2}) + \mathcal{O}(s^{b+1}) = \mathcal{O}(s^\ell), \end{aligned}$$

where $\ell \geq m$. For any $m > 2$, since $\mathcal{O}(s^{a+2}) \leq \mathcal{O}(s^3)$, we must have $b = 1$ to cancel out the $\mathcal{O}(s^2)$ terms in the last step of the above equality.

Similarly, to see the relation between c and d, we have

$$\begin{aligned} P_{\mathcal{N}_2}F([w;\nu]) &= \sum_{j=c}^{n}\frac{1}{j+1}C_{(j)}([w;\nu])e_{w\nu} + \sum_{j=d}^{n}\frac{1}{j+1}D_{(j)}([w;\nu])e_{w\nu} + \mathcal{O}(\|e_{w\nu}\|^{n+2}) \\ &= \mathcal{O}(s^{c+2}) + \mathcal{O}(s^{d+1}) + \mathcal{O}(s^{n+2}) = \mathcal{O}(s^m). \end{aligned} \tag{4.17}$$

Clearly, (4.17) holds only if exactly one of the following cases is true:

1. If $c \geq m-1$, then we must have $d = m-1$ ($m \geq 2$) to maintain a $\mathcal{O}(s^m)$ term on the left-hand side of (4.17).
2. If $c = m-2$, then we must have $d \geq m-1$ ($m \geq 3$, $b = 1$) so that there is no term of order lower than m on the left-hand side of (4.17).
3. If $c \leq m-3$, then we must have $d = c+1$ ($m \geq 4$, $b = 1$) so that the two terms of order lower than m on the left-hand side of (4.17) are cancelled out.

The lemma is thus established. □

Lemma 4.7 completes step 1, where we derived the possible values of b, c, and d for the Taylor expansion of $F([w;\nu])$ at $[v;\lambda]$. In step 2, we show that all the half-step and full-step iterates of the accelerated inverse iteration are well-defined. To this end, it is sufficient to show that the Jacobian of Newton's method at any half-step or full-step eigenpair approximation $[w;\nu]$ or $[x;\mu]$ is nonsingular. The nonsingularity of the Jacobian can be guaranteed by the following Lemma.

LEMMA 4.8. *Let $[x;\mu]$ be an eigenpair approximation sufficiently close, but not equal to $[v;\lambda]$. Then $F'([x;\mu]) = \begin{bmatrix} T(\mu) & T'(\mu)x \\ u^* & 0 \end{bmatrix}$, the Jacobian of Newton's method at $[x;\mu]$, is nonsingular.*

Proof. By assumption, the eigenvalues of $T(\cdot)$ are isolated, and therefore $T(\mu)$ is nonsingular if μ is sufficiently close, but not equal to λ. It follows that $\begin{bmatrix} T(\mu) \\ u^* \end{bmatrix}$ has full column rank. Assume that the Jacobian $\begin{bmatrix} T(\mu) & T'(\mu)x \\ u^* & 0 \end{bmatrix}$ is singular, then there exists $y \in \mathbb{C}^n$ such that $\begin{bmatrix} T(\mu) \\ u^* \end{bmatrix} y = \begin{bmatrix} T'(\mu)x \\ 0 \end{bmatrix}$. It follows that $y = T(\mu)^{-1}T'(\mu)x$ and $u^*y = 0$. However, if x is sufficiently close to v in direction, and $|\mu-\lambda|$ sufficiently small, then y, the unnormalized new eigenvector approximation, is closer to v in direction. Given the normalization condition $u^*v = 1$, it is impossible to have $u^*y = 0$. Therefore the Jacobian must be nonsingular. □

In step 3, we first show that the error of the full-step iterate can be written as a linear combination of the half-step iterate error and the errof of the next standard Newton iterate $[z;\xi] = [w;\nu] - F'([w;\nu])^{-1}F([w;\nu])$; this derivation follows that in

[8, Section 4]. Then, we study the projections of the full-step iterate error onto $\mathcal{N}_1$ and $\mathcal{M}_1$, and show that the projected errors are bounded by $\mathcal{O}(s^2)$.

To decompose the error of the full-step iterate, define

$$[z;\xi] = [w;\nu] - F'([w;\nu])^{-1}F([w;\nu]),$$

the iterate obtained by applying one step of Newton's method to the half-step iterate. Then we have from (4.11) that $[x_{k+1};\mu_{k+1}] = m[z;\,\xi] - (m-1)[w;\nu]$. The error of $[x_{k+1};\mu_{k+1}]$ can be analyzed by studying $e_{z\xi} = [z;\,\xi] - [v;\lambda]$. Following the derivation in [8, Section 4], one can show that $e_{z\xi}$ satisfies

$$\begin{aligned}(4.18)\qquad e_{z\xi} &= e_{w\nu} - F'([w;\nu])^{-1}F([w;\nu])\\ &= F'([w;\nu])^{-1}\Big\{\sum_{j=a}^{n}\frac{j}{(j+1)}A_{(j)}([w;\nu])e_{w\nu} + \sum_{j=b}^{n}\frac{j}{(j+1)}B_{(j)}([w;\nu])e_{w\nu}\\ &\qquad \sum_{j=c}^{n}\frac{j}{(j+1)}C_{(j)}([w;\nu])e_{w\nu} + \sum_{j=d}^{n}\frac{j}{(j+1)}D_{(j)}([w;\nu])e_{w\nu} + \mathcal{O}(s^{n+2})\Big\}.\end{aligned}$$

To study the errors of $[x_{k+1};\mu_{k+1}]$ projected onto $\mathcal{N}_1$ and $\mathcal{M}_1$, we assume that the first case discussed in Lemma 4.7 holds, that is, $c \geq d = m-1$; we assume in addition that $\bar{c} \geq \bar{d}$. These assumptions are similar, but not identical, to those in [8, Section 7]. Since $P_{\mathcal{M}_1}e_{w\nu} = \mathcal{O}(s^2)$ and $P_{\mathcal{N}_1}e_{w\nu} = \mathcal{O}(s)$, we have

$$\begin{aligned}(4.19)\quad [x_{k+1};\mu_{k+1}] - [v;\lambda] &= m[z;\,\xi] - (m-1)[w;\nu] - [v;\lambda] = me_{z\xi} - (m-1)e_{w\nu}\\ &= mF'([w;\nu])^{-1}\Big\{\frac{a}{a+1}A_{(a)}([w;\nu])e_{w\nu} + \frac{b}{b+1}B_{(b)}([w;\nu])e_{w\nu} + \frac{c}{c+1}C_{(c)}([w;\nu])e_{w\nu}\\ &\quad + \frac{d}{d+1}D_{(d)}([w;\nu])e_{w\nu} + P_{\mathcal{M}_2}\mathcal{O}(s^{\min(a+3,b+2)}) + P_{\mathcal{N}_2}\mathcal{O}(s^{\min(c+3,d+2)})\Big\}\\ &\quad -(m-1)F'([w;\nu])^{-1}F'([w;\nu])e_{w\nu}\\ &= F'([w;\nu])^{-1}\Big\{-(m-1)A_{F^*}e_{w\nu} + \Big(\frac{ma}{a+1} - (m-1)\Big)A_{(a)}([w;\nu])e_{w\nu} +\\ &\quad \Big(\frac{mb}{b+1} - (m-1)\Big)B_{(b)}([w;\nu])e_{w\nu} + P_{\mathcal{M}_2}\mathcal{O}(s^{\min(a+3,b+2)}) + P_{\mathcal{N}_2}\mathcal{O}(s^{d+2})\Big\}.\end{aligned}$$

Here, in the last step of (4.19), $C_{(c)}([w;\nu])e_{w\nu} = C_{(c)}([w;\nu])(P_{\mathcal{M}_1}e_{w\nu}) = P_{\mathcal{N}_2}\mathcal{O}(s^{c+2})$ does not appear explicitly, because it is assimilated into $P_{\mathcal{N}_2}\mathcal{O}(s^{d+2})$, where $d \leq c$. More importantly, as $d = m-1$ by our assumption, $D_{(d)}([w;\nu])e_{w\nu}$ vanishes because its coefficient is $m\frac{d}{d+1} - (m-1) = 0$. The cancellation of $D_{(d)}([w;\nu])e_{w\nu}$ is critical in the proof of the quadratic convergence of the accelerated method.

To finish step 3, we show that the errors of $[x_{k+1};\mu_{k+1}]$ projected onto $\mathcal{N}_1$ and $\mathcal{M}_1$ are both bounded by $\mathcal{O}(s^2)$. To this end, recall from (2.19) the expression of $F'([w;\nu])^{-1}$, and apply it to (4.19). With some algebraic manipulation, we have

$$[x_{k+1};\mu_{k+1}] - [v;\lambda] \equiv e^{k+1}_{\mathcal{M}\mathcal{M}} + e^{k+1}_{\mathcal{M}\mathcal{N}} + e^{k+1}_{\mathcal{N}\mathcal{M}} + e^{k+1}_{\mathcal{N}\mathcal{N}},$$

where

$$
\begin{aligned}
e^{k+1}_{\mathcal{M}\mathcal{M}} &= P_{\mathcal{M}_1}\big\{A_F^{-1}([w;\nu]) + A_F^{-1}([w;\nu])B_F([w;\nu])S_F^{-1}([w;\nu])C_F([w;\nu])A_F^{-1}([w;\nu])\big\}\\
&\quad\times\Big\{-(m-1)A_{F^*}e_{w\nu} + \frac{a+1-m}{a+1}A_{(a)}([w;\nu])e_{w\nu} + \frac{b+1-m}{b+1}B_{(b)}([w;\nu])e_{w\nu}\\
&\quad + P_{\mathcal{M}_2}\mathcal{O}(s^{\min(a+3,b+2)})\Big\},\\
e^{k+1}_{\mathcal{M}\mathcal{N}} &= -P_{\mathcal{M}_1}A_F^{-1}([w;\nu])B_F([w;\nu])S_F^{-1}([w;\nu])P_{\mathcal{N}_2}\mathcal{O}(s^{d+2}),\\
e^{k+1}_{\mathcal{N}\mathcal{M}} &= -P_{\mathcal{N}_1}S_F^{-1}([w;\nu])C_F([w;\nu])A_F^{-1}([w;\nu])P_{\mathcal{M}_2}\Big\{-(m-1)A_{F^*}e_{w\nu} +\\
&\quad \frac{a+1-m}{a+1}A_{(a)}([w;\nu])e_{w\nu} + \frac{b+1-m}{b+1}B_{(b)}([w;\nu])e_{w\nu} + P_{\mathcal{M}_2}\mathcal{O}(s^{\min(a+3,b+2)})\Big\},
\end{aligned}
$$

and $e^{k+1}_{\mathcal{N}\mathcal{N}} = P_{\mathcal{N}_1}S_F^{-1}([w;\nu])P_{\mathcal{N}_2}\mathcal{O}(s^{d+2})$.

We show that all the projected errors shown above are bounded by $\mathcal{O}(s^2)$. First, note from (2.20) that the dominant term of $A_F([w;\nu])$ is $A_{F^*} = P_{\mathcal{M}_2}F'([v;\lambda])P_{\mathcal{M}_1}$, which means $\|A_F([w;\nu])\| = \mathcal{O}(1)$ and $\|A_F^{-1}([w;\nu])\| = \mathcal{O}(1)$. In addition, by (2.18), we have $\|S_F([w;\nu])\| = \mathcal{O}(s^{\min(\bar{d},\bar{b}+\bar{c})})$. Thus the operator involved in $e^{k+1}_{\mathcal{M}\mathcal{M}}$ satisfies

$$
\begin{aligned}
&\|A_F^{-1}([w;\nu]) + A_F^{-1}([w;\nu])B_F([w;\nu])S_F^{-1}([w;\nu])C_F([w;\nu])A_F^{-1}([w;\nu])\|\\
&\le \mathcal{O}(1) + \mathcal{O}(s^{\bar{b}+\bar{c}-\min(\bar{d},\bar{b}+\bar{c})}) \le \mathcal{O}(1) + \mathcal{O}(1) = \mathcal{O}(1).
\end{aligned}
$$

It follows that $\|e^{k+1}_{\mathcal{M}\mathcal{M}}\| = \mathcal{O}(1)\big(\mathcal{O}(s^2) + \mathcal{O}(s^{a+2}) + \mathcal{O}(s^{b+1})\big) = \mathcal{O}(s^2)$.

For the second error term $e^{k+1}_{\mathcal{M}\mathcal{N}}$, since $\bar{c} \ge \bar{d}$ by our assumption, we have

$$
\|A_F^{-1}([w;\nu])B_F([w;\nu])S_F^{-1}([w;\nu])\| \le \mathcal{O}(s^{\bar{b}-\min(\bar{d},\bar{b}+\bar{c})}) = \mathcal{O}(s^{\bar{b}-\bar{d}}),
$$

and it follows that $\|e^{k+1}_{\mathcal{M}\mathcal{N}}\| \le \mathcal{O}(s^{\bar{b}-\bar{d}})\mathcal{O}(s^{d+2}) \le \mathcal{O}(s^{\bar{b}+2})$.

Similarly, for the third error term $e^{k+1}_{\mathcal{N}\mathcal{M}}$, we have

$$
\|S_F^{-1}([w;\nu])C_F([w;\nu])A_F^{-1}\| \le \mathcal{O}(s^{\bar{c}-\min(\bar{d},\bar{b}+\bar{c})}) = \mathcal{O}(s^{\bar{c}-\bar{d}}),
$$

and therefore $\|e^{k+1}_{\mathcal{N}\mathcal{M}}\| \le \mathcal{O}(s^{\bar{c}-\bar{d}})\big(\mathcal{O}(s^2) + \mathcal{O}(s^{a+2}) + \mathcal{O}(s^{b+1})\big) \le \mathcal{O}(s^2)$.

Finally, the last error term $e^{k+1}_{\mathcal{N}\mathcal{N}}$ can be directly bounded by $\|S_F^{-1}([w;\nu])\|$:

$$
\|e^{k+1}_{\mathcal{N}\mathcal{N}}\| \le \mathcal{O}(s^{-\min(\bar{d},\bar{b}+\bar{c})})\mathcal{O}(s^{d+2}) = \mathcal{O}(s^{-\bar{d}+d+2}) \le \mathcal{O}(s^2).
$$

The above analysis completes step 3, and the result is summarized as follows.

THEOREM 4.9. *Let λ be a defective eigenvalue of the holomorphic matrix pencil T with one left and one right Jordan chains of length m, and $v = \varphi_{1,0}$ be the corresponding eigenvector. Let $\delta, \theta > 0$ be some appropriately small constants, $[x_0;\mu_0] \in W(\delta,\theta)$ be an eigenpair approximation of $[v;\lambda]$ satisfying Assumption* 4.4. *Under Assumption* 4.6, *suppose that for any half-step iterate $[w_k;\nu_k]$, $\bar{c} \ge \bar{d}$, and $c \ge d = m-1$. Then for sufficiently small* $\sin\angle(x_0, v)$, *the full-step iterates of the accelerated method* (4.11) (or (4.12)) *are well-defined, and $[x_k;\mu_k]$ converges towards $[v;\lambda]$ quadratically.*

Remark. One can see from the above derivation that $c \ge d = m-1$ and $\bar{c} \ge \bar{d}$ are critical assumptions leading to the quadratic convergence of the accelerated methods. In addition, $[x_{k+1};\mu_{k+1}] = m\big([w;\nu] - F'([w;\nu])^{-1}F([w;\nu])\big) - (m-1)[w;\nu]$ is the unique linear combination of the two iterates that cancels out the error terms lying

in $\mathcal{N}_1$ on the order of $\mathcal{O}(s)$. A violation of these assumptions or a different linear combination would lead to a deceleration of the convergence rate back to linear.

Theorem 4.9 is an extension of the major results in [8, Section 7] to the special setting of eigenvalue computation under less stringent assumptions. Specifically, [8] studied two accelerated Newton's methods for solving a general nonlinear system of equations for a singular root. It was assumed there that $a = \bar{a}, b = \bar{b}, c = \bar{c}$ and $d = \bar{d}$ for any intermediate and full step iterates. Under certain additional hypothesis, the first accelerated method requires the computation of three Newton's directions per iteration, assuming that $c \geq d$ and $b \geq \min(2, d)$; the second one solves for two Newton's directions per iteration, assuming that $b \geq 2$ and $c \geq d \geq 2$. In fact, for the computation of degenerate eigenvalues discussed here, these hypotheses do not hold. Our assumption in Theorem 4.9 about the values of $c, d, \bar{c}$, and $\bar{d}$ is made for the half-step iterate $[w; \nu]$ alone, and it is less demanding than those in [8].

4.5.2. Accelerated single-vector JD. One could also design other accelerated Newton-like methods from the accelerated inverse iteration (4.12). In this section, we propose an accelerated single-vector JD, which is derived from a minor modification of (4.12). The only difference between the two algorithms lies in the computation of new eigenvalue approximations. In contrast to Newton's method and RFI, the JD methods compute *normalized* new eigenvector approximations directly without forming the *unnormalized* version; as a result, the way the accelerated Newton's method updates eigenvalue approximations cannot be realized by JD; see Steps 3 and 6 in (4.12). To work around this difficulty, we use the Rayleigh functional value as new eigenvector approximations, and we have the new algorithm as follows:

$$
\left\{
\begin{array}{l}
\text{1. Choose vector } y_k, \text{ e.g., } y_k = T'(\mu_k)x_k, \text{ define } \Pi_k^{(1)} = I - \dfrac{T'(\mu_k)x_k y_k^*}{y_k^* T'(\mu_k)x_k}, \\
\quad \Pi_k^{(2)} = I - \dfrac{x_k u^*}{u^* x_k}, \text{ and solve the correction equation} \\
\quad \Pi_k^{(1)} T(\mu_k) \Pi_k^{(2)} \Delta x_k = -\left(T(\mu_k) - \dfrac{y_k^* T(\mu_k) x_k}{y_k^* T'(\mu_k) x_k} T'(\mu_k) \right) x_k \text{ for } \Delta x_k \perp u; \\
\text{2. } w_k = x_k + \Delta x_k; \\
\text{3. Choose vector } z_{k1}, \text{e.g., } z_{k1} = T'(\mu_k) w_k \text{ and compute the RF value} \\
\quad \nu_k = \rho_F(w_k; T, z_{k1}); \\
\text{4. Define } \widetilde{\Pi}_k^{(1)} = I - \dfrac{T'(\nu_k) w_k z_{k1}^*}{z_{k1}^* T'(\nu_k) w_k}, \widetilde{\Pi}_k^{(2)} = I - \dfrac{w_k u^*}{u^* w_k}, \text{ and solve the} \\
\quad \text{correction equation } \widetilde{\Pi}_k^{(1)} T(\nu_k) \widetilde{\Pi}_k^{(2)} \Delta w_k = -T(\nu_k) w_k \text{ for } \Delta w_k \perp u; \\
\text{5. } x_{k+1} = -(m-1) w_k + m(w_k + \Delta w_k) = w_k + m \Delta w_k; \\
\text{6. Choose vector } z_{k2}, \text{e.g., } z_{k2} = T'(\nu_k) x_{k+1} \text{ and compute the RF value} \\
\quad \mu_{k+1} = \rho_F(x_{k+1}; T, z_{k2}).
\end{array}
\right. \tag{4.20}
$$

Following the standard derivation of the exact solution of JD correction equations, we can show that $\Delta x_k = \dfrac{T^{-1}(\mu_k)T'(\mu_k)x_k}{u^* T^{-1}(\mu_k)T'(\mu_k)x_k} - x_k$ at Step 1 of (4.20), and thus $w_k = \dfrac{T^{-1}(\mu_k)T'(\mu_k)x_k}{u^* T^{-1}(\mu_k)T'(\mu_k)x_k}$ at Step 2; similarly, $\Delta w_k = \dfrac{T^{-1}(\nu_k)T'(\nu_k)w_k}{u^* T^{-1}(\nu_k)T'(\nu_k)w_k} - w_k$ at Step 4, and $x_{k+1} = \dfrac{m T^{-1}(\nu_k)T'(\nu_k)w_k}{u^* T^{-1}(\nu_k)T'(\nu_k)w_k} - (m-1)w_k$ at Step 5. Assuming x_0 is normalized such that $u^* x_0 = 1$, then all the following half-step and full-step eigenvector

approximations satisfy $u^*w_k = u^*x_{k+1} = 1$. For the purpose of numerical stability, however, we recommend these conditions to be explicitly enforced at Steps 2 and 5.

We see that the only difference between the accelerated inverse iteration (4.12) and the accelerated single-vector JD (4.20) is the way new eigenvalue approximations are computed. Consequently, algorithms (4.20) and (4.11) are not mathematically equivalent. Nevertheless, given the close similarity between the two methods, it is natural to expect that the accelerated JD exhibits quadratic convergence for defective eigenpairs. This convergence rate is illustrated by numerical experiments.

4.6. Numerical experiments for the accelerated algorithms. We present numerical results for the accelerated inverse iteration and the accelerated JD on the problems with a single Jordan chain, namely, *time_delay* and *jordan*3. We run the accelerated algorithms with an initial eigenpair approximation and we find that both converge superlinearly. To illustrate the order of convergence descriptively, we follow the approach used in Section 3.2: a sequence of initial approximations $(\mu_0^{(j)}, x_0^{(j)})$ is generated, then one step of the accelerated algorithms is applied to obtain a sequence of new approximations $(\mu_1^{(j)}, x_1^{(j)})$, and an estimate of the order of convergence ℓ is obtained by analyzing $\left(\log e_0^{(j)}, \log e_1^{(j)}\right)$. The results presented in Table 4.4 show that both algorithms converge quadratically for the test problems.

		accelerated inverse iter.		accelerated JD	
problem	$\angle(x_0^{(1)}, v)$	# init. approx.	est. ℓ	# init. approx.	est. ℓ
time_delay	10^{-3}	18	2.011	11	2.032
*jordan*3	2.5×10^{-3}	9	2.028	9	2.058

TABLE 4.4
Estimated order of convergence of the accelerated algorithms for a defective λ ($geo_T(\lambda) = 1$)

4.7. Defective eigenvalues with multiple Jordan chains. We studied in Sections 4.3 and 4.5 the convergence of several Newton-like methods for a defective eigenvalue λ with a single Jordan chain ($J \equiv geo_T(\lambda) = 1$). To make our discussion more complete, we consider in this section defective eigenvalues with multiple ($J \geq 2$) Jordan chains. For this type of eigenvalues with certain simple spectral structures, we can develop a detailed convergence analysis as we did for those with a single Jordan chain. Due to the limit of space, however, we would not pursue such a thorough investigation in this paper; instead, we provide some heuristic insight into the convergence rates the Newton-like methods are most likely to exhibit. Our speculation is directly based on the results developed for defective λ with $J = 1$, and we will later illustrate our discussion by numerical experiments.

Let λ be a defective eigenvalue of the holomorphic $T(\cdot)$ with $J = geo_T(\lambda) \geq 2$, and $\{\{\varphi_{1,0}, \ldots, \varphi_{1,m_1-1}\}, \{\varphi_{2,0}, \ldots, \varphi_{2,m_2-1}\} \ldots, \{\varphi_{J,0}, \ldots, \varphi_{J,m_J-1}\}\}$ be the corresponding Jordan chains. Assume without loss of generality that $m_1 \leq m_2 \leq \ldots \leq m_J$. We consider several types of spectral structure as follows.

Case 1: $m_1 \geq 2$**.** One may call this type of eigenvalue "purely defective" since it can be considered as a combination of several defective eigenpairs sharing the same eigenvalue, each of which has a single Jordan chain of length $m_i \geq 2$. In this case, we have shown in Section 4.1 that the standard inverse iteration converges linearly. In addition, if each Jordan chain satisfies the assumption of Theorem 4.3, it is natural to expect the local convergence of RFI and single-vector JD to be linear in general.

To achieve quadratic convergence, we may use the two accelerated algorithms

(4.12) and (4.20) with $m = m_J$ used for the linear combination to construct the full-step iterates. The motivation for choosing this value for m is as follows. As the Newton-like methods proceed, the eigenvector approximation x_k tends to converge towards the eigenspace spanned by eigenvectors associated with the longest Jordan chains. In fact, assume without loss of generality that $J = 2$ and $2 \le m_1 < m_2$. Let (μ, x) be the current eigenpair approximation. The new eigenvector approximation is

$$p = T^{-1}(\mu)T'(\mu)x = \sum_{k=1}^{2}\sum_{j=0}^{m_k-1}\sum_{i=0}^{m_k-j-1}\frac{\langle T'(\mu)x,\psi_{k,j}\rangle}{(\mu-\lambda)^{m_k-j-i}}\varphi_{k,i} + G(\mu)T'(\mu)x \tag{4.21}$$

$$= \sum_{i=0}^{m_1-1}\frac{\langle T'(\mu)x,\psi_{1,0}\rangle}{(\mu-\lambda)^{m_1-i}}\varphi_{1,i} + \sum_{j=1}^{m_1-1}\sum_{i=0}^{m_1-j-1}\frac{\langle T'(\mu)x,\psi_{1,j}\rangle}{(\mu-\lambda)^{m_1-j-i}}\varphi_{1,i} +$$

$$\sum_{i=0}^{m_2-1}\frac{\langle T'(\mu)x,\psi_{2,0}\rangle}{(\mu-\lambda)^{m_2-i}}\varphi_{2,i} + \sum_{j=1}^{m_2-1}\sum_{i=0}^{m_2-j-1}\frac{\langle T'(\mu)x,\psi_{2,j}\rangle}{(\mu-\lambda)^{m_2-j-i}}\varphi_{2,i} + G(\mu)T'(\mu)x.$$

Assume that $\langle T''(\lambda)\varphi_{1,0},\psi_{2,0}\rangle \neq 0$ and $\langle T''(\lambda)\varphi_{2,0},\psi_{2,0}\rangle \neq 0$, or $\langle T'(\lambda)\varphi_{1,0},\psi_{2,1}\rangle \neq 0$ and $\langle T'(\lambda)\varphi_{2,0},\psi_{2,1}\rangle \neq 0$. Following the proof of Lemma 4.5, we can show that the dominant term in (4.21) can be written as $\mathcal{O}\left((\mu-\lambda)^{-(m_2-1)}\right)\varphi_{2,0}$. In other words, the new eigenvector approximation contains little component of $\varphi_{1,0}$, and Newton-like methods behave as if there is only one Jordan chain $\{\varphi_{2,0},\ldots,\varphi_{2,m_2-1}\}$ involved. Thus we expect the accelerated algorithms with $m = m_2$ to converge quadratically.

Case 2: $m_1 = 1$ **and** $m_J \ge 3$**.** In this case, it is not difficult to follow the idea given in Section 4.1 to show that inverse iteration converges linearly. In addition, for any practical Newton-like methods where the new eigenvector approximation is $p = T^{-1}(\mu)T'(\mu)x$, one can show that p is dominated by a term of the form $\mathcal{O}\left((\mu-\lambda)^{-(m_J-1)}\right)\varphi_{J,0}$, and p contains another term of the form $\mathcal{O}\left((\mu-\lambda)^{-1}\right)\varphi_{1,0}$. Assume again without loss of generality that $J = 2$. Since $m_2 \ge 3$, the dominant term in p is much larger in magnitude than the $\varphi_{1,0}$ term. As a result, the Jordan chain of length 1 has minimal impact on the algorithm, and Newton-like methods should behave the same way as they do for Case 1.

Case 3: $m_1 = 1$ **and** $m_J = 2$**.** The linear convergence of inverse iteration can be established as in Section 4.1. For other Newton-like methods, this case seems more complicated than the previous two because it is not clear whether these algorithms converge to the eigenspace associated with the short ($m_i = 1$) or the long ($m_i = 2$) Jordan chains. In fact, the new eigenvector approximation $p = T^{-1}(\mu)T'(\mu)x$ contains both $\mathcal{O}\left((\mu-\lambda)^{-1}\right)\varphi_{1,0}$ and $\mathcal{O}\left((\mu-\lambda)^{-1}\right)\varphi_{J,0}$, and p is not necessarily dominated by either of the two components. We do not have a complete understanding of the convergence of Newton-like methods for this case, but we will discuss two numerical examples in the next section.

4.8. Numerical experiments for defective eigenvalues with multiple Jordan chains. In this section, we provide numerical evidence to illustrate our heuristic analysis of the convergence of Newton-like methods for defective eigenvalues with multiple Jordan chains. Four problems, namely, *df_art_m1m2*, *df_art_m1m3*, *df_art_m2m3*, and *mirror* (see Section 3.2) are used to test the convergence rates. As we discussed, we first run the algorithms with an initial eigenpair (μ_0, x_0) and see how quickly $\|T(\mu_k)x_k\|$ decreases to determine if the convergence is linear or at least superlinear. For algorithms that seem to converge linearly and superlinearly, respectively, we follow the standard approach (see Section 4.2 for defective eigenval-

ues) and the more descriptive approach (see Section 3.2 for semi-simple eigenvalues) to estimate the order of convergence.

		inverse iteration		RFI/JD		TSRFI	
problem	$\angle(x_0, v)$	# iters	est. ℓ	# iters	est. ℓ	# iters	est. ℓ
df_art_m1m3	10^{-2}	14	0.978	14	0.957	10	0.965*
df_art_m2m3	10^{-2}	15	0.969	14	0.974	11	1.013*
df_art_m1m2	5×10^{-2}	17	1.000	12	0.984	8	0.973*
mirror	10^{-2}	15	1.002	3	$\approx 2^{\dagger}$	2	$\approx 3^{\dagger}$

TABLE 4.5

Estimated order of convergence of the non-accelerated algorithms for a defective λ ($geo_T(\lambda) \geq 2$)

The results for inverse iteration, RFI/JD, and TSRFI are presented in Table 4.5. We see that inverse iteration converges linearly for all problems, and RFI and TSRFI also converge linearly for the three artificially constructed problems. The problem *mirror* is the only one with defective eigenvalues in our tests for which RFI and TSRFI exhibit the same order of convergence as for simple and semi-simple eigenvalues. We do not have a complete understanding of this observation, but we find that the desired eigenvalue $\lambda = 0$ of this problem has a special spectrum structure. Namely, it has two Jordan chains of length 2, and seven Jordan chains of length 1; for the two longest Jordan chains $\{\varphi_{1,0}, \varphi_{1,1}\}$ and $\{\varphi_{2,0}, \varphi_{2,1}\}$, it holds that $\text{span}\{\varphi_{1,0}, \varphi_{2,0}\} = \text{span}\{\varphi_{1,1}, \varphi_{2,1}\}$; that is, the generalized eigenvectors and the eigenvectors of these Jordan chains span the same space. We speculate that the special spectral structure plays a critical role in the high order of convergence.

		accelerated inverse iter.		accelerated JD	
problem	$\angle(x_0^{(1)}, v)$	# init. approx.	est. ℓ	# init. approx.	est. ℓ
df_art_m1m3	2.5×10^{-2}	11	1.998	10	2.010
df_art_m2m3	5×10^{-3}	8	2.015	8	2.014
problem	$\angle(x_0, v)$	# iters.	est. ℓ	# iters.	est. ℓ
df_art_m1m2	10^{-1}	9	1.054	3	≈ 2
mirror	10^{-2}	3	≈ 2	3	≈ 2

TABLE 4.6

Estimated order of convergence of accelerated algorithms for defective λ ($geo_T(\lambda) \geq 2$)

Table 4.6 summarizes the estimated order of convergence of the accelerated algorithms. For both algorithms, the parameter m is set to be the length of the longest Jordan chains. We see that the accelerated algorithms generally exhibit quadratic convergence for defective eigenvalues with multiple Jordan chains, with the only exception that the accelerated inverse iteration converges linearly for *df_art_m1m2*. This problem belongs to Case 3 discussed in Section 4.7, for which our understanding of the convergence of Newton-like methods is not complete. Nevertheless, Tables 4.4 and 4.6 show that the accelerated JD converges quadratically for all test problems.

In fact, for some reason, our approach used in Section 3.2 does not give a descriptive estimate of the true order of convergence of the accelerated algorithms for *df_art_m1m2* and *mirror*. Note that *mirror* also belongs to Case 3 discussed in Section 4.7. To estimate the true order of convergence, we ran the algorithms with

*The residual norms in the first two iterations are not used for the estimate of order of convergence for TSRFI, because they decrease much less rapidly in subsequent iterations.

†For the problem *mirror*, one can see by the standard criterion $\|e_{k+1}\|/\|e_k\|^{\ell} \leq C$ that RFI and TSRFI, respectively, exhibit quadratic and cubic convergence; our approach used in Section 3.2 somehow does not generate a descriptive estimate of the order of convergence for this problem.

(μ_0, x_0) and then used the standard criterion $\|e_{k+1}\|/\|e_k\|^\ell \le C$. For these two problems, we speculate that the eigenpair approximations generated by the accelerated algorithms have certain special structure for which our approach used in Section 3.2 fails to detect the actual rate at which $\|T(\mu_k)x_k\|$ decreases*.

5. Conclusion. The local convergence of single-vector Newton-like methods for degenerate eigenvalues has not been fully understood, since the standard convergence theory of Newton's method based on the nonsingularity of the Jacobian is not applicable in this setting. In this paper, we studied the convergence of several of the most widely-used single-vector Newton-like methods for the solution of a degenerate eigenvalue and a corresponding eigenvector of general nonlinear algebraic eigenvalue problems of the form $T(\lambda)v = 0$. Our major conclusion is that at least quadratic convergence can be achieved by these algorithms for both semi-simple and defective eigenvalues.

Specifically, we showed that Newton-like methods exhibit the same order of convergence for semi-simple eigenvalues as they do for simple eigenvalues. The convergence is generally quadratic; in addition, RFI/JD with appropriate use of the Rayleigh functional can achieve cubic convergence for problems with local symmetry.

The convergence analysis for defective eigenvalues is more complicated. We showed the linear convergence of inverse iteration and RFI/JD, and we proposed two accelerated algorithms which converge quadratically for a defective λ with a single Jordan chain. We also gave some heuristic discussion on the convergence for a defective λ with multiple Jordan chains. Our analyses are illustrated by numerical experiments.

REFERENCES

[1] J. Asakura, T. Sakurai, H. Tadano, T. Ikegami and K. Kimura, *A numerical method for polynomial eigenvalue problems using contour integral*, Japan Journal of Industrial and Applied Mathematics, Volume 27 (2010), pp. 73–90.

[2] T. Betcke, N. J. Higham, V. Mehrmann, C. Schröder and F. Tisseur, *NLEVP: a collection of nonlinear eigenvalue problems*, MIMS EPrint 2010.98, Manchester Institute for Mathematical Sciences, University of Manchester, 2010.

[3] T. Betcke and D. Kressner, *Perturbation, extraction and refinement of invariant pairs for matrix polynomials*, Linear Algebra and its Applications, Vol. 435 (2011), pp. 514–536.

[4] T. Betcke and H. Voss, *A Jacobi-Davidson type projection method for nonlinear eigenvalue problems*, Future Generation Comuter Systems, Vol. 20 (2004), pp. 363–372.

[5] W.-J. Beyn, *An integral method for solving nonlinear eigenvalue problems*, Linear Algebra and its Applications, Vol. 436 (2012), pp. 3839–3863.

[6] D. W. Decker and C. T. Kelley, *Newton's method at singular points I*, SIAM Journal on Numerical Analysis, Vol. 17 (1980), pp. 66–70.

[7] D. W. Decker and C. T. Kelley, *Newton's method at singular points II*, SIAM Journal on Numerical Analysis, Vol. 17 (1980), pp. 465–471.

[8] D. W. Decker, H. B. Keller and C. T. Kelley, *Convergence rates for Newton's method at singular points*, SIAM Journal on Numerical Analysis, Vol. 20 (1983), pp. 296–314.

[9] N. Hale, N. J. Higham, L. N. Trefethen, *Computing A^α, $\log(A)$, and related matrix functions by contour integrals*, SIAM Journal on Numerical Analysis, Vol. 46 (2008), pp. 2505–2523.

[10] I. C. F. Ipsen, *Computing an eigenvector with inverse iteration*, SIAM Review, Vol. 39 (1997), pp. 254–291.

*A similar example: our approach used in Section 3.2, when applied to inverse iteration for computing defective eigenvalues with a single Jordan chain, gives an estimated mth order convergence, which does not reflect the actual linear convergence; this is due to the special structure of the new iterate generated by inverse iteration; see Lemma 4.5.

[11] E. Jarlebring and W. Michiels, *Analyzing the convergence factor of residual inverse iteration*, BIT Numerical Mathematics, Vol. 51(2011), pp. 937–957.
[12] V. Kozlov and V. Maz'ia, *Differential equations with operator coefficients*, Springer, Berlin-Heidelberg, 1999.
[13] D. Kressner, *A block Newton method for nonlinear eigenvalue problems*, Numerische Mathematik, Vol. 114 (2009), pp. 355–372.
[14] D.S. Mackey, N. Mackey, C. Mehl and V. Mehrmann, *Vector spaces of linearizations for matrix polynomials*, SIAM Journal Matrix Analysis and Applications, Vol. 28 (2006), pp. 971–1004.
[15] D.S. Mackey, N. Mackey, C. Mehl and V. Mehrmann, *Structured polynomial eigenvalue problems: good vibrations from good linearizations*, SIAM Journal Matrix Analysis and Applications, Vol. 28 (2006), pp. 1029–1051.
[16] The Matrix Market, *http://math.nist.gov/MatrixMarket/*, NIST, 2007.
[17] V. Mehrmann and C. Schröder, *Nonlinear eigenvalue and frequency response problems in industrial practice*, Journal of Mathematics in Industry, Vol. 1 (2011), article No. 7.
[18] V. Mehrmann and H. Voss, *Nonlinear eigenvalue problems: a challenge for modern eigenvalue methods*, Mitteilungen der Gesellschaft für Angewandte Mathematik und Mechanik, Vol. 27 (2005), pp. 121–151.
[19] J. Moro, J. V. Burke and M. L. Overton, *On the Lidskii–Vishik–Lyusternik perturbation theory for eigenvalues of matrices with arbitrary Jordan structure*, SIAM Journal Matrix Analysis and Applications, Vol. 18 (1997), pp. 793–817.
[20] J. Moro and F.M. Dopico, *First Order Eigenvalue Perturbation Theory and the Newton Diagram*, Chapter in the book *Applied Mathematics and Scientific Computing*, edited by Z. Drmac, V. Hari, L. Sopta, Z. Tutek and K. Veselic, pp. 143–175. Kluwer Academic Publishers (2003).
[21] A. Neumaier, *Residual inverse iteration for the nonlinear eigenvalue problem*, SIAM Journal on Numerical Analysis, Vol. 22 (1985), pp. 914–923.
[22] M.R. Osborne, *Inverse iteration, Newton's method, and non-linear eigenvalue problems*, The Contributions of Dr. J.H. Wilkinson to Numerical Analysis, Symposium Proceedings Series, 19, pp. 21–53, The Institute of Mathematics and its Applications, London, 1979.
[23] G. Peters and J. H. Wilkinson, *Inverse iteration, ill-conditioned equations and Newton's method*, SIAM Review, Vol. 21 (1979), pp. 339–360.
[24] A. Ruhe, *Algorithms for the nonlinear eigenvalue problem*, SIAM Journal on Numerical Analysis, Vol. 10 (1973), pp. 674–689.
[25] K. Schreiber, *Nonlinear eigenvalue problems: Newton-type methods and nonlinear Rayleigh functionals*, Ph.D thesis, Department of Mathematics, TU Berlin, 2008.
[26] H. Schwetlick and K. Schreiber, *Nonlinear Rayleigh functionals*, Linear Algebra and Its Applications, Vol. 436 (2012), pp. 3991–4016.
[27] A. Spence and C. Poulton, *Photonic band structure calculations using nonlinear eigenvalue techniques*, Journal of Computational Physics, Vol. 204 (2005), pp. 65–81.
[28] Y. Su and Z. Bai, *Solving Rational Eigenvalue Problems via Linearization*, SIAM Journal Matrix Analysis and Applications, Vol. 32 (2011), pp. 201–216.
[29] D. B. Szyld and F. Xue, *Local convergence analysis of several inexact Newton-type algorithms for general nonlinear eigenvalue problems*, to appear in Numerische Mathematik.
[30] D. B. Szyld and F. Xue, *Several properties of invariant pairs of nonlinear algebraic eigenvalue problems*, Temple Research Report 12-02-09, February 2012.
[31] F. Tisseur and K. Meerbergen, *The quadratic eigenvalue problem*, SIAM Review, Vol. 43 (2001), pp. 234–286.