Robust successive computation of eigenpairs for nonlinear eigenvalue problems

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Newton-based methods are well-established techniques for solving nonlinear eigenvalue problems. If, however, a larger portion of the spectrum is sought, their tendency to reconverge to previously determined eigenpairs is a hindrance. To overcome this limitation, we propose and analyze a deflation strategy for nonlinear eigenvalue problems, based on the concept of minimal invariant pairs. We develop this strategy into a Jacobi-Davidson-type method and discuss its various algorithmic details. Finally, the efficiency of our approach is demonstrated by a sequence of numerical examples.

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1 Introduction

We consider nonlinear eigenvalue problems of the form

$$T(\lambda)x = 0, \qquad x \neq 0 \tag{1}$$

with a matrix-valued function $T : \Omega \to \mathbb{C}^{n\times n}$, which is holomorphic on some subdomain $\Omega \subset \mathbb{C}$ of the complex plane. We confine ourselves to regular nonlinear eigenvalue problems, i.e., problems for which $\det T(\lambda)$ does not vanish identically. Any pair (x, λ) satisfying (1) is called an eigenpair of T, consisting of the eigenvector x and the eigenvalue λ.

Nonlinear eigenvalue problems of the aforementioned form arise in a variety of applications, such as photonic bandstructure calculation [10], vibrational simulation of fluid-solid structures [37, 36], electromagnetic modeling of particle accelerators [22], computational quantum chemistry [39], or stability analysis of time-delay systems [27, 15]. In finite-element discretizations of operator eigenvalue problems, nonlinearities are often caused by λ-dependent material parameters [28], λ-dependent boundary conditions [8, 26], or the use of special basis functions [5, 19]. Boundary-element discretizations, on the other hand, can lead to nonlinear eigenvalue problems even if the underlying operator eigenvalue problem is linear [34]. For a more comprehensive overview of sources for nonlinear eigenvalue problems of type (1), see [25] or [4].

A number of algorithms for the solution of the nonlinear eigenvalue problem (1) can be found in the literature; see [25, 31] for a survey of classical methods and [38, 40, 20, 6, 18] for more recent developments. Unfortunately, most available techniques are single-vector iterations and therefore directed towards computing one eigenpair only. The robust and reliable calculation of several eigenpairs—although required by many applications—is much more difficult and less well studied.

Essentially, there appear to be two different strategies: The desired eigenpairs can be computed either simultaneously or successively. The simultaneous computation of eigenpairs can be achieved by deriving block versions of the aforementioned single-vector iterations. In [20], minimal invariant pairs are introduced as a numerically robust means of representing several eigenpairs and a block Newton method is constructed to compute them. However, the resulting methods are harder to analyze and seem to be more restrictive in terms of local convergence than their single-vector counterparts. Moreover, the number of eigenpairs to be approximated must be known in advance.

In contrast, computing eigenpairs successively avoids all of the above disadvantages. In particular, convergence can be monitored and steered much more easily for individual eigenpairs than for blocks. However, one has to ensure that the algorithm does not repeatedly converge to the same eigenpair. In principle, this issue could be addressed by keeping a list of previously converged eigenpairs and then discarding further copies as they arise but such a strategy seems impractical for several reasons. First of all, it does not save the computational work spent on recomputing eigenpairs. More importantly, it is likely to cause difficulties in the presence of multiple or nearly-multiple eigenvalues.

A much more preferable solution would be to deflate converged eigenpairs from the problem as this reliably prevents reconvergence and tends to enlarge the convergence basin for unconverged eigenpairs. This is a well-known technique for linear eigenvalue problems [11, 21, 35, 2], where the fact that their eigenvectors are linearly independent is exploited to accomplish the deflation via partial Schur forms. In the context of nonlinear eigenvalue problems, though, linear independence of the eigenvectors is no longer guaranteed and insisting that the computed eigenvectors be linearly independent therefore bears the danger of missing eigenpairs.

Existing deflation strategies for nonlinear eigenvalue problems are based on computing partial Schur forms of related linear eigenvalue problems; see [24, 16] for examples. In the present paper, we propose a deflation strategy operating on the original nonlinear formulation of the problem. The algorithm to be developed computes several eigenpairs successively but represents them together as a single invariant pair. By maintaining the minimality of this invariant pair, we prevent the algorithm from reconverging to the same eigenpairs while retaining the favorable convergence properties of single-vector iterations. Multiple or even defective eigenvalues, on the other hand, are detected and the correct number of copies is retrieved.

The remainder of this paper is organized as follows. After reviewing the concept of invariant pairs in Section 2, the deflation strategy is developed in Section 3. In Section 4, a Newton method employing the deflation strategy is constructed and turned into a Jacobi-Davidson-type algorithm by complementing it with subspace acceleration techniques. A sequence of numerical experiments in Section 5 demonstrates the efficiency of the presented algorithm.

2 Minimal invariant pairs

Minimal invariant pairs [20] generalize the notion of invariant subspaces to the nonlinear setting. They provide a means to represent several eigenpairs of a nonlinear eigenvalue problem in a numerically robust way and hence constitute a fundamental ingredient for the upcoming developments.

The concept can be motivated as follows. Since the matrix-valued function T is assumed to be holomorphic, the nonlinear eigenvalue problem (1) can be rewritten using the Cauchy integral formula as

$$T(\lambda)x = \frac{1}{2\pi \mathrm{i}} \int_{\partial B_\delta(\lambda)} T(z)x(z-\lambda)^{-1}\,\mathrm{d}z = 0, \tag{2}$$

where $B_\delta(\lambda)$ denotes the ball of radius δ around λ and $\delta > 0$ is chosen such that $B_\delta(\lambda) \subset \Omega$. The formulation (2) of the nonlinear eigenvalue problem has the advantage that it naturally extends into a block version. Hence, we are led to the subsequent definition.

Definition 2.1. $(X, \Lambda) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ is called an invariant pair of the nonlinear eigenvalue problem (1) if and only if the block residual defined via

$$\mathbf{T}(X, \Lambda) := \frac{1}{2\pi \mathrm{i}} \int_\Gamma T(z)X(zI - \Lambda)^{-1}\,\mathrm{d}z \tag{3}$$

is equal to zero. Here, Γ is a contour (i.e., a simply closed curve) in Ω enclosing the eigenvalues of Λ in its interior. Note that such a contour Γ always exists because the eigenvalues of Λ are isolated points in Ω.

The contour integral formulation (3) of the block residual is the most suitable one for our theoretical derivations. However, alternative characterizations do exist. Most notably, in applications, T often takes the form $T(\lambda) = f_1(\lambda)T_1 + \cdots + f_d(\lambda)T_d$ with constant coefficient matrices $T_1, \ldots, T_d$ and scalar, holomorphic functions $f_1, \ldots, f_d$. It has been shown in [7] that in this case, the definition of $\mathbf{T}(X, \Lambda)$ in (3) is equivalent to

$$\mathbf{T}(X, \Lambda) = T_1 X f_1(\Lambda) + \cdots + T_d X f_d(\Lambda), \tag{4}$$

which is more useful for computations. Here, $f_j(\Lambda)$ is to be understood as a matrix function in the sense of [14].

As is easily seen, an invariant pair (X, Λ) with $m = 1$ (i.e., X is a vector and Λ a scalar) amounts to an eigenpair, provided that $X \neq 0$. In case $m > 1$, a similar connection can be established in that for every eigenpair (u, λ) of Λ, (Xu, λ) is an eigenpair of the nonlinear eigenvalue problem (1), provided that $Xu \neq 0$. The latter condition can be rephrased as requiring that $u = 0$ be the only null vector of the augmented matrix

$$\begin{bmatrix} X \\ \Lambda - \lambda I \end{bmatrix}. \tag{5}$$

This justifies the following definition.

Definition 2.2. A pair (X, Λ) is called minimal if and only if the matrix in (5) has full column rank for all eigenvalues λ of Λ or, equivalently, for all $\lambda \in \mathbb{C}$.

A different but equivalent characterization of minimality has been given in [20]. It is summarized by the following lemma.

Lemma 2.3. *A pair $(X, \Lambda) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ is minimal if and only if there exists an integer ℓ such that the matrix*

$$\mathbf{V}_\ell(X, \Lambda) = \begin{bmatrix} X \\ X\Lambda \\ \vdots \\ X\Lambda^{\ell-1} \end{bmatrix} \tag{6}$$

has full column rank.

Lemma 2.3 is a well-known result in mathematical systems theory, where the stated equivalence is exploited in the Hautus test [13] for observability of a matrix pair. In this setting, (5) and (6) correspond to the Hautus and Kalman observability matrices, respectively. The application of this result to minimal pairs is due to [7]. The smallest integer ℓ for which $\mathbf{V}_\ell(X, \Lambda)$ in (6) has full column rank is called the minimality index of a minimal pair (X, Λ) in [20].

Typically, the minimality index of a minimal pair $(X, \Lambda) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ is quite small. Generically, it is equal to one unless $m > n$. For larger minimality indices, though, the monomials Λ^i, $i = 0, \ldots, \ell - 1$ within the matrix $\mathbf{V}_\ell(X, \Lambda)$ may cause numerical instabilities. This effect can be mitigated by replacing the monomials with a different polynomial basis.

Lemma 2.4. *A pair $(X, \Lambda) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ is minimal of index at most ℓ if and only if the matrix*

$$\mathbf{V}_\ell^p(X, \Lambda) = \begin{bmatrix} Xp_0(\Lambda) \\ \vdots \\ Xp_{\ell-1}(\Lambda) \end{bmatrix} \tag{7}$$

has full column rank, where the polynomials $p_0, \ldots, p_{\ell-1}$ constitute a basis for the vector space of polynomials of degree at most $\ell - 1$.

Proof. Let the polynomials $p_0, \ldots, p_{\ell-1}$ be an arbitrary basis for the space of polynomials of degree at most $\ell - 1$ and let

$$p_i(\lambda) = p_{i,0} + p_{i,1} \cdot \lambda + \cdots + p_{i,\ell-1} \cdot \lambda^{\ell-1}, \qquad i = 0, \ldots, \ell - 1$$

be their expansion with respect to the monomial basis. Then the matrix

$$P = \begin{bmatrix} p_{0,0} & \cdots & p_{0,\ell-1} \\ \vdots & \ddots & \vdots \\ p_{\ell-1,0} & \cdots & p_{\ell-1,\ell-1} \end{bmatrix},$$

and hence also $P \otimes I$, is nonsingular. The claimed equivalence is established by noticing that $\mathbf{V}_\ell^p(X, \Lambda) = (P \otimes I)\mathbf{V}_\ell(X, \Lambda)$ with $\mathbf{V}_\ell(X, \Lambda)$ and $\mathbf{V}_\ell^p(X, \Lambda)$ as defined in (6) and (7), respectively. □

As noted in [20], invariance and minimality of a pair are preserved under a certain kind of transformation. The details are covered by the next lemma.

Lemma 2.5. *Let $(X, \Lambda) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$. Then for any invertible matrix J,*

$$\mathbf{T}(XJ, J^{-1}\Lambda J) = \mathbf{T}(X, \Lambda)J \qquad \text{and} \qquad \mathbf{V}_\ell^p(XJ, J^{-1}\Lambda J) = \mathbf{V}_\ell^p(X, \Lambda)J.$$

In particular, if (X, Λ) is invariant and/or minimal, then so is $(XJ, J^{-1}\Lambda J)$.

Proof. The first formula is immediately clear from the definition (3) of the block residual $\mathbf{T}$. The second formula is a consequence of the well-known fact that $p_i(J^{-1}\Lambda J) = J^{-1}p_i(\Lambda)J$, $i = 0, \ldots, \ell-1$. From these formulas it is obvious that $\mathbf{T}(X, \Lambda) = 0$ implies $\mathbf{T}(XJ, J^{-1}\Lambda J) = 0$ and $\mathbf{V}_\ell^p(XJ, J^{-1}\Lambda J)$ has full column rank if and only if the same is true of $\mathbf{V}_\ell^p(X, \Lambda)$, thereby proving the last statement. □

3 Robust expansion of invariant pairs

Suppose that a minimal invariant pair $(X, \Lambda) \in \mathbb{C}^{n\times m} \times \mathbb{C}^{m\times m}$ of the nonlinear eigenvalue problem (1) is known. The aim of this section is to extend (X, Λ) into a minimal invariant pair $(\hat{X}, \hat{\Lambda})$ of larger size. Employing the ansatz

$$(\hat{X}, \hat{\Lambda}) = \left(\begin{bmatrix} X & y \end{bmatrix}, \begin{bmatrix} \Lambda & v \\ 0 & \mu \end{bmatrix} \right) \in \mathbb{C}^{n\times(m+1)} \times \mathbb{C}^{(m+1)\times(m+1)}, \tag{8}$$

our goal becomes the determination of $y \in \mathbb{C}^n$, $v \in \mathbb{C}^m$, and $\mu \in \Omega$ such that the pair $(\hat{X}, \hat{\Lambda})$ is both invariant and minimal. This strategy can be seen as the nonlinear counterpart to expanding a partial Schur decomposition, such as in the Jacobi-Davidson QR and QZ methods [11].

Throughout this section, Γ denotes a contour in Ω, enclosing both the eigenvalues of Λ and μ in its interior. The following lemma gives a necessary and sufficient condition for the invariance of the pair $(\hat{X}, \hat{\Lambda})$.

Lemma 3.1. *Let (X, Λ) be an invariant pair of the nonlinear eigenvalue problem (1). Then the extended pair $(\hat{X}, \hat{\Lambda})$ defined in (8) is invariant if and only if*

$$T(\mu)y + U(\mu)v = 0, \tag{9}$$

where

$$U(\mu) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma T(z)X(zI - \Lambda)^{-1}(z - \mu)^{-1}\, \mathrm{d}z. \tag{10}$$

Proof. Recall that $(\hat{X}, \hat{\Lambda})$ is invariant if and only if $\mathbf{T}(\hat{X}, \hat{\Lambda}) = 0$ with $\mathbf{T}$ as defined in (3). Since

$$(zI - \hat{\Lambda})^{-1} = \begin{bmatrix} (zI - \Lambda)^{-1} & (zI - \Lambda)^{-1}v(z - \mu)^{-1} \\ 0 & (z - \mu)^{-1} \end{bmatrix},$$

we have

$$\mathbf{T}(\hat{X}, \hat{\Lambda}) = \begin{bmatrix} \mathbf{T}(X, \Lambda) & T(\mu)y + U(\mu)v \end{bmatrix}.$$

Hence, the condition $\mathbf{T}(\hat{X}, \hat{\Lambda}) = 0$ decomposes into (9) as well as $\mathbf{T}(X, \Lambda) = 0$. The proof is concluded by noticing that the latter equation will always be satisfied since (X, Λ) constitutes an invariant pair. □

Note that the left-hand side of Equation (9) is linear in both y and v; the dependence on μ is nonlinear but holomorphic as the subsequent result shows.

Lemma 3.2. *U as defined in (10) depends holomorphically on μ.*

Proof. The differentiability of U is evident from its contour integral representation (10). The k-th derivative is given by

$$U^{(k)}(\mu) = \frac{k!}{2\pi \mathrm{i}} \int_\Gamma T(z)X(zI - \Lambda)^{-1}(z - \mu)^{-(k+1)}\, \mathrm{d}z. \qquad \square$$

Assume we have found $(y, v, \mu) \in \mathbb{C}^n \times \mathbb{C}^m \times \Omega$ such that the condition (9) is met. The next result states a necessary and sufficient criterion for the minimality of the ensuing augmented pair $(\hat{X}, \hat{\Lambda})$.

Lemma 3.3. *Let the pair (X, Λ) be minimal of index ℓ and let the polynomials $p_0, \dots, p_\ell$, given by*

$$p_i(\lambda) = (\alpha_{i,1}\lambda - \beta_{i,1}) \cdots (\alpha_{i,d_i}\lambda - \beta_{i,d_i}), \qquad i = 0, \dots, \ell,$$

constitute a basis for the vector space of polynomials of degree at most ℓ. Then the extended pair $(\hat{X}, \hat{\Lambda})$ defined in (8) is minimal if and only if

$$\mathbf{v}(y, v, \mu) \notin \operatorname{span} \mathbf{V}_{\ell+1}^p(X, \Lambda) \tag{11}$$

with $\mathbf{V}_{\ell+1}^p(X, \Lambda)$ as defined in (7) and

$$\mathbf{v}(y, v, \mu) = \begin{bmatrix} p_0(\mu)y + Xq_0(\mu)v \\ \vdots \\ p_\ell(\mu)y + Xq_\ell(\mu)v \end{bmatrix}, \tag{12}$$

where the polynomials $q_0, \dots, q_\ell$ are defined by

$$q_i(\mu) = \sum_{j=1}^{d_i} (\alpha_{i,1}\Lambda - \beta_{i,1}I) \cdots (\alpha_{i,j-1}\Lambda - \beta_{i,j-1}I)\alpha_{i,j}(\alpha_{i,j+1}\mu - \beta_{i,j+1}) \cdots (\alpha_{i,d_i}\mu - \beta_{i,d_i}).$$

In particular, if the extended pair $(\hat{X}, \hat{\Lambda})$ is minimal, its minimality index cannot exceed $\ell + 1$.

Proof. To show the statement about the minimality index, consider the degree-graded, monic polynomials $\tilde{p}_i(\lambda) = (\lambda - \mu)^i$, $i = 0, \dots, \ell$. One readily verifies that these polynomials constitute a basis for the vector space of polynomials of degree at most ℓ and that the matrix $\mathbf{V}_{\ell+1}^{\tilde{p}}(\hat{X}, \hat{\Lambda})$ defined as in (7) is given by

$$\mathbf{V}_{\ell+1}^{\tilde{p}}(\hat{X}, \hat{\Lambda}) = \begin{bmatrix} X & y \\ \mathbf{V}_\ell(X, \Lambda) \cdot (\Lambda - \mu I) & \mathbf{V}_\ell(X, \Lambda) \cdot v \end{bmatrix} = \begin{bmatrix} I & \\ & \mathbf{V}_\ell(X, \Lambda) \end{bmatrix} \begin{bmatrix} X & y \\ \Lambda - \mu I & v \end{bmatrix}$$

with $\mathbf{V}_\ell(X, \Lambda)$ as in (6). The first matrix in the product on the right has full column rank thanks to the minimality of (X, Λ). If the extended pair $(\hat{X}, \hat{\Lambda})$ is minimal, by Definition 2.2 with $\lambda = \mu$, also the second matrix in the product, and hence $\mathbf{V}_{\ell+1}^{\tilde{p}}(\hat{X}, \hat{\Lambda})$, has full column rank. Therefore, by Lemma 2.4, the minimality index of $(\hat{X}, \hat{\Lambda})$ is at most $\ell + 1$.

Using the knowledge about the minimality index, the extended pair $(\hat{X}, \hat{\Lambda})$ is minimal by Lemma 2.4 if and only if $\mathbf{V}_{\ell+1}^p(\hat{X}, \hat{\Lambda})$ has full column rank. A straightforward calculation reveals that $\mathbf{V}_{\ell+1}^p(\hat{X}, \hat{\Lambda}) = \left[\mathbf{V}_{\ell+1}^p(X, \Lambda), \mathbf{v}(y, v, \mu)\right]$ with $\mathbf{v}(y, v, \mu)$ as defined in (12). Since by minimality of (X, Λ), $\mathbf{V}_{\ell+1}^p(X, \Lambda)$ already has full column rank, the assertion follows. □

To enforce criterion (11) within a computational method, we impose the stronger condition

$$\mathbf{v}(y, v, \mu) \perp \operatorname{span} \mathbf{V}_{\ell+1}^p(X, \Lambda), \qquad \mathbf{v}(y, v, \mu) \neq 0.$$

The orthogonality requirement amounts to $\left[\mathbf{V}_{\ell+1}^p(X, \Lambda)\right]^{\mathsf{H}} \mathbf{v}(y, v, \mu) = 0$. By inserting the definitions of $\mathbf{V}_{\ell+1}^p(X, \Lambda)$ and $\mathbf{v}(y, v, \mu)$ in (7) and (12), respectively, this can be rewritten as

$$A(\mu)y + B(\mu)v = 0 \tag{13}$$

with the polynomials

$$\begin{aligned} A(\mu) &= p_0(\mu) \cdot p_0(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} + \cdots + p_\ell(\mu) \cdot p_\ell(\Lambda)^{\mathsf{H}} X^{\mathsf{H}}, \\ B(\mu) &= p_0(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} X q_0(\mu) + \cdots + p_\ell(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} X q_\ell(\mu). \end{aligned} \tag{14}$$

The non-degeneracy condition $\mathbf{v}(y, v, \mu) \neq 0$ is simplified by the subsequent lemma.

Lemma 3.4. *Let the pair (X, Λ) be minimal of index ℓ and let $\mathbf{v}(y, v, \mu)$ be defined as in (12). Then $\mathbf{v}(y, v, \mu) = 0$ if and only if $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right] = 0$.*

Proof. From the definition of $\mathbf{v}(y, v, \mu)$, it is obvious that $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right] = 0$ entails $\mathbf{v}(y, v, \mu) = 0$. For the converse, assume that $\mathbf{v}(y, v, \mu) = 0$ and define the polynomials $\tilde{p}_i(\lambda) = (\lambda - \mu)^i$, $i = 0, \ldots, \ell$. Let

$$\tilde{p}_i(\lambda) = \tilde{p}_{i,0} \cdot p_0(\lambda) + \cdots + \tilde{p}_{i,\ell} \cdot p_\ell(\lambda), \qquad i = 0, \ldots, \ell$$

be the expansion of the $\tilde{p}_i$ in the polynomial basis formed by $p_0, \ldots, p_\ell$. Introducing the matrix $\tilde{P} = \left[\tilde{p}_{i,j}\right]_{i=0,\ldots,\ell}^{j=0,\ldots,\ell}$, one calculates that

$$0 = (\tilde{P} \otimes I) \cdot \mathbf{v}(y, v, \mu) = \begin{bmatrix} y \\ \mathbf{V}_\ell(X, \Lambda) v \end{bmatrix},$$

which implies $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right] = 0$ because $\mathbf{V}_\ell(X, \Lambda)$ as defined in (6) has full column rank thanks to the minimality of (X, Λ). □

Combining the invariance condition (9), the minimality condition (13), and the simplified non-degeneracy condition from Lemma 3.4, we obtain

$$\begin{bmatrix} T(\mu) & U(\mu) \\ A(\mu) & B(\mu) \end{bmatrix} \begin{bmatrix} y \\ v \end{bmatrix} = 0, \qquad \begin{bmatrix} y \\ v \end{bmatrix} \neq 0. \tag{15}$$

Note that (15) again has the structure of a nonlinear eigenvalue problem. This nonlinear eigenvalue problem is of size $(n + m) \times (n + m)$, where $n \times n$ is the size of the original eigenproblem and m is the size of the existing minimal invariant pair $(X, \Lambda) \in \mathbb{C}^{n \times m} \times \mathbb{C}^{m \times m}$. Since m can be expected to be quite small compared to n, the increase in size is only marginal.

By solving the nonlinear eigenvalue problem (15), we obtain $y \in \mathbb{C}^n$, $v \in \mathbb{C}^m$, and $\mu \in \Omega$ needed to extend the existing minimal invariant pair (X, Λ) via (8). Clearly, the matrix-valued function in (15) is holomorphic since this is true for each of its blocks: $T(\mu)$ is holomorphic by assumption, the holomorphy of $U(\mu)$ has been shown in Lemma 3.2, and $A(\mu)$, $B(\mu)$ are just polynomials. Thus, any technique for solving holomorphic nonlinear eigenvalue problems can be applied to (15).

The subsequent theorem, which is the main theoretical result of this work, states that by solving the eigenvalue problem (15) instead of (1), we indeed deflate the invariant pair (X, Λ) from the computation.

Theorem 3.5. *Let (X, Λ) be a minimal invariant pair of the regular nonlinear eigenvalue problem (1). If $\left(\left[\begin{smallmatrix} Y \\ V \end{smallmatrix}\right], M\right)$ is a minimal invariant pair of the augmented nonlinear eigenvalue problem (15), then $\left([X, Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right)$ is a minimal invariant pair of the original nonlinear eigenvalue problem (1). Conversely, if $\left([X, Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right)$ is a minimal invariant pair of the original nonlinear eigenvalue problem (1), then there exists a unique matrix F such that $\left(\left[\begin{smallmatrix} Y - XF \\ V - (\Lambda F - FM) \end{smallmatrix}\right], M\right)$ is a minimal invariant pair of the augmented nonlinear eigenvalue problem (15). In particular, if the eigenproblem (1) is regular, then the augmented eigenproblem (15) is regular as well.*

Proof. Let $p_0, \dots, p_\ell$ be the polynomial basis used for the definition of $A(\mu)$, $B(\mu)$ in (14) and let the polynomials $q_0, \dots, q_\ell$ be defined correspondingly as in Lemma 3.3. Furthermore, let $\mathcal{C}$ be a contour in Ω, enclosing the eigenvalues of M in its interior, and define

$$\mathbf{U}(V,M) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} U(\xi) V (\xi I - M)^{-1} \,\mathrm{d}\xi, \qquad \mathbf{q}_i(V,M) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} q_i(\xi) V (\xi I - M)^{-1} \,\mathrm{d}\xi,$$
$$\mathbf{A}(Y,M) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} A(\xi) Y (\xi I - M)^{-1} \,\mathrm{d}\xi, \qquad \mathbf{B}(V,M) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} B(\xi) V (\xi I - M)^{-1} \,\mathrm{d}\xi.$$

W.l.o.g. we may choose the contour $\mathcal{C}$ such that it does not pass through any eigenvalues of Λ. Then it follows from Lemma 4.2 below that

$$\mathbf{U}(V,M) = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} T(\xi) X (\xi I - \Lambda)^{-1} V (\xi I - M)^{-1} \,\mathrm{d}\xi.$$

Employing the definitions of the polynomials $A(\mu)$ and $B(\mu)$ in (14), we find

$$\mathbf{A}(Y,M) = p_0(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} Y p_0(M) + \cdots + p_\ell(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} Y p_\ell(M),$$
$$\mathbf{B}(V,M) = p_0(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} X \mathbf{q}_0(V,M) + \cdots + p_\ell(\Lambda)^{\mathsf{H}} X^{\mathsf{H}} X \mathbf{q}_\ell(V,M).$$

Thus, by summing up,

$$\mathbf{A}(Y,M) + \mathbf{B}(V,M) = \mathbf{V}_{\ell+1}^{p}(X,\Lambda)^{\mathsf{H}} \cdot \begin{bmatrix} Y p_0(M) + X \mathbf{q}_0(V,M) \\ \vdots \\ Y p_\ell(M) + X \mathbf{q}_\ell(V,M) \end{bmatrix} \tag{16}$$

with $\mathbf{V}_{\ell+1}^{p}(X,\Lambda)$ defined as in (7).

We now turn to the first statement of the theorem. Suppose that the pair $\left(\left[\begin{smallmatrix} Y \\ V \end{smallmatrix}\right], M\right)$ is invariant with respect to the augmented nonlinear eigenvalue problem (15). By Definition 2.1, this is equivalent to

$$0 = \frac{1}{2\pi\mathrm{i}} \int_{\mathcal{C}} \begin{bmatrix} T(\xi) & U(\xi) \\ A(\xi) & B(\xi) \end{bmatrix} \begin{bmatrix} Y \\ V \end{bmatrix} (\xi I - M)^{-1} \,\mathrm{d}\xi = \begin{bmatrix} \mathbf{T}(Y,M) + \mathbf{U}(V,M) \\ \mathbf{A}(Y,M) + \mathbf{B}(V,M) \end{bmatrix}. \tag{17}$$

In order to prove the invariance of the extended pair $\left([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right)$, we need to show that $\mathbf{T}\left([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right) = 0$ with $\mathbf{T}$ as defined in (3). Exploiting

$$\left(zI - \begin{bmatrix} \Lambda & V \\ 0 & M \end{bmatrix} \right)^{-1} = \begin{bmatrix} (zI - \Lambda)^{-1} & (zI - \Lambda)^{-1} V (zI - M)^{-1} \\ 0 & (zI - M)^{-1} \end{bmatrix}$$

together with the block structure of the extended pair, we find

$$\mathbf{T}\left([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right) = \begin{bmatrix} \mathbf{T}(X,\Lambda) & \mathbf{T}(Y,M) + \mathbf{U}(V,M) \end{bmatrix}. \tag{18}$$

The first block row of Equation (17) shows that the second component on the right-hand side of the last equation is zero. The first component vanishes because (X,Λ) is invariant, implying the invariance of $\left([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right)$ as claimed.

To conclude that $\left([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\right)$ is minimal, we have to demonstrate that for any $\lambda \in \mathbb{C}$, the equation

$$\begin{bmatrix} X & Y \\ \Lambda - \lambda I & V \\ 0 & M - \lambda I \end{bmatrix} \begin{bmatrix} g \\ h \end{bmatrix} = 0 \tag{19}$$

admits only the trivial solution $\left[\begin{smallmatrix} g \\ h \end{smallmatrix}\right] = 0$. Note that any solution of Equation (19) satisfies

$$\begin{bmatrix} X & Y \end{bmatrix} \begin{bmatrix} g \\ h \end{bmatrix} = 0, \qquad \begin{bmatrix} \Lambda & V \\ 0 & M \end{bmatrix} \begin{bmatrix} g \\ h \end{bmatrix} = \lambda \begin{bmatrix} g \\ h \end{bmatrix},$$

implying $\mathbf{V}_{\ell+1}^p\big([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\big)\left[\begin{smallmatrix} g \\ h \end{smallmatrix}\right] = 0$. Premultiplying the last equation by $\mathbf{V}_{\ell+1}^p(X,\Lambda)^{\mathsf{H}}$ and exploiting the block structure of $\mathbf{V}_{\ell+1}^p\big([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\big)$ as well as Equation (16), we obtain

$$\begin{aligned} 0 &= \mathbf{V}_{\ell+1}^p(X,\Lambda)^{\mathsf{H}} \cdot \mathbf{V}_{\ell+1}^p\big([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\big)\left[\begin{smallmatrix} g \\ h \end{smallmatrix}\right] \\ &= \big[\mathbf{V}_{\ell+1}^p(X,\Lambda)^{\mathsf{H}} \cdot \mathbf{V}_{\ell+1}^p(X,\Lambda)\big] \cdot g + \big[\mathbf{A}(Y,M) + \mathbf{B}(V,M)\big] \cdot h. \end{aligned}$$

Because of the second block row in Equation (17), the summand involving h disappears, entailing $g = 0$ since the matrix $\mathbf{V}_{\ell+1}^p(X,\Lambda)^{\mathsf{H}} \cdot \mathbf{V}_{\ell+1}^p(X,\Lambda)$ is positive definite. Hence, Equation (19) reduces to

$$\begin{bmatrix} Y \\ V \\ M - \lambda I \end{bmatrix} h = 0, \tag{20}$$

which has only the solution $h = 0$ as a result of the minimality of $\big(\left[\begin{smallmatrix} Y \\ V \end{smallmatrix}\right], M\big)$. This finishes the proof of the first statement.

For the converse statement, assume that $\big([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\big)$ is a minimal invariant pair of the original nonlinear eigenvalue problem (1). As an immediate consequence, the pair $\big(\left[\begin{smallmatrix} Y \\ V \end{smallmatrix}\right], M\big)$ is minimal because for any solution h of Equation (20), $\left[\begin{smallmatrix} 0 \\ h \end{smallmatrix}\right]$ is a solution of Equation (19) and therefore zero.

From the calculation in Equation (17), it is clear that the pair $\big(\left[\begin{smallmatrix} Y \\ V \end{smallmatrix}\right], M\big)$ is invariant if the conditions

$$\mathbf{T}(Y,M) + \mathbf{U}(V,M) = 0 \qquad \text{and} \qquad \mathbf{A}(Y,M) + \mathbf{B}(V,M) = 0$$

hold. The first condition follows directly from the invariance of $\big([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\big)$ via Equation (18). The second condition, however, need not be satisfied in general.

Instead of $\big([X,Y], \left[\begin{smallmatrix} \Lambda & V \\ 0 & M \end{smallmatrix}\right]\big)$, we can also apply the above arguments starting from the transformed pair

$$\begin{bmatrix} X & Y \end{bmatrix} \begin{bmatrix} I & F \\ 0 & I \end{bmatrix}^{-1} = \begin{bmatrix} X & Y - XF \end{bmatrix}, \quad \begin{bmatrix} I & F \\ 0 & I \end{bmatrix} \begin{bmatrix} \Lambda & V \\ 0 & M \end{bmatrix} \begin{bmatrix} I & F \\ 0 & I \end{bmatrix}^{-1} = \begin{bmatrix} \Lambda & V - (\Lambda F - FM) \\ 0 & M \end{bmatrix},$$

which is minimal and invariant by Lemma 2.5, regardless of the choice of the matrix F. This yields that the pair $\big(\left[\begin{smallmatrix} Y - XF \\ V - (\Lambda F - FM) \end{smallmatrix}\right], M\big)$ is minimal and satisfies the first condition required for invariance. The second condition required for invariance of this pair reads

$$\mathbf{A}(Y - XF, M) + \mathbf{B}(V - (\Lambda F - FM), M) = 0$$

and the proof of the converse statement is completed by determining F such that this condition is fulfilled. Applying (16), the condition can be rearranged into

$$\mathbf{V}_{\ell+1}^p(X,\Lambda)^{\mathsf{H}} \begin{bmatrix} XFp_0(M) + X\mathbf{q}_0(\Lambda F - FM, M) \\ \vdots \\ XFp_\ell(M) + X\mathbf{q}_\ell(\Lambda F - FM, M) \end{bmatrix} = \mathbf{V}_{\ell+1}^p(X,\Lambda)^{\mathsf{H}} \begin{bmatrix} Yp_0(M) + X\mathbf{q}_0(V, M) \\ \vdots \\ Yp_\ell(M) + X\mathbf{q}_\ell(V, M) \end{bmatrix}.$$

Because $\Lambda F - FM = (\Lambda - \xi I)F + F(\xi I - M)$, we have for $i = 0, \ldots, \ell$,

$$\mathbf{q}_i(\Lambda F - FM, M) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} q_i(\xi)(\Lambda - \xi I)F(\xi I - M)^{-1} \, \mathrm{d}\xi + \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} q_i(\xi) F \, \mathrm{d}\xi.$$

The second summand on the right-hand side vanishes since the integrand is a polynomial and hence holomorphic. For the first summand, a telescoping sum argument gives $q_i(\xi)(\Lambda - \xi I) = p_i(\Lambda) - p_i(\xi)I$. The resulting relation $\mathbf{q}_i(\Lambda F - FM, M) = p_i(\Lambda)F - Fp_i(M)$ simplifies the second invariance condition above to

$$\left[\mathbf{V}_\ell^p(X, \Lambda)^{\mathsf{H}} \mathbf{V}_\ell^p(X, \Lambda)\right] F = \mathbf{V}_\ell^p(X, \Lambda)^{\mathsf{H}} \begin{bmatrix} Y p_0(M) + X \mathbf{q}_0(V, M) \\ \vdots \\ Y p_\ell(M) + X \mathbf{q}_\ell(V, M) \end{bmatrix}.$$

Since the matrix $\mathbf{V}_\ell^p(X, \Lambda)^{\mathsf{H}} \mathbf{V}_\ell^p(X, \Lambda)$ is positive definite thanks to the minimality of (X, Λ), there exists a unique matrix F such that this condition is satisfied.

Finally, we prove the statement about the regularity by contradiction. To this end, assume that the augmented problem is singular, i.e., it has an eigenpair, or in other words, a minimal invariant pair $\left(\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right], \mu\right)$, for every $\mu \in \Omega$. As shown before, the extended pair $(\hat{X}, \hat{\Lambda})$ in (8) is then minimal and invariant with respect to the original problem. Obviously, μ is an eigenvalue of $\hat{\Lambda}$. Let u be a corresponding eigenvector, then $(\hat{X}u, \mu)$ is an eigenpair of the original problem. Since $\mu \in \Omega$ can be chosen arbitrarily, the original problem is singular, in contradiction to the hypothesis. □

4 Algorithmic realization

In the following, we will derive an algorithm to efficiently solve the augmented nonlinear eigenvalue problems of the form (15) arising from the deflation strategy in the previous section. We begin by constructing a (simplified) Newton method and then turn this method into a Jacobi-Davidson-type algorithm by adding subspace acceleration as well as inexact solves of the correction equation. In this context, it will again be more convenient to consider the first and second block row of (15) individually.

4.1 A Newton approach

Assume we already have an approximate solution $(y, v, \mu) \in \mathbb{C}^n \times \mathbb{C}^m \times \Omega$ in our hands and want to compute a correction $(\triangle y, \triangle v, \triangle \mu)$ such that $(y + \triangle y, v + \triangle v, \mu + \triangle \mu)$ is an even better approximation. Ideally, the update leads to the exact solution, i.e.,

$$\begin{bmatrix} T(\mu + \triangle \mu) & U(\mu + \triangle \mu) \\ A(\mu + \triangle \mu) & B(\mu + \triangle \mu) \end{bmatrix} \begin{bmatrix} y + \triangle y \\ v + \triangle v \end{bmatrix} = 0. \tag{21}$$

To avoid the degenerate solution $\triangle y = -y, \triangle v = -v$, we additionally impose the orthogonality constraint

$$\begin{bmatrix} y \\ v \end{bmatrix}^{\mathsf{H}} \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} = 0. \tag{22}$$

Let σ be a shift close to the target eigenvalue. Employing Taylor expansion and neglecting higher order terms, (21) becomes

$$\begin{bmatrix} r \\ s \end{bmatrix} + \triangle \mu \begin{bmatrix} \dot{r} \\ \dot{s} \end{bmatrix} + \begin{bmatrix} T(\sigma) & U(\sigma) \\ A(\sigma) & B(\sigma) \end{bmatrix} \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} + (\mu + \triangle \mu - \sigma) \begin{bmatrix} \dot{T}(\sigma) & \dot{U}(\sigma) \\ \dot{A}(\sigma) & \dot{B}(\sigma) \end{bmatrix} \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} = 0, \tag{23}$$

Algorithm 1: A simplified Newton method for solving the augmented nonlinear eigenvalue problem (15).

Input: minimal invariant pair (X, Λ), initial approximation (y_0, v_0, μ_0)
Output: solution (y, v, μ) of (15)

determine minimality index ℓ of (X, Λ)
for $k = 0, 1, 2, \ldots$ *until convergence* **do**
  pick a shift $\sigma = \sigma_k$
  solve the correction equation (25) for $\triangle y$, $\triangle v$, $\triangle \mu$
  $y_{k+1} = y_k + \triangle y$
  $v_{k+1} = v_k + \triangle v$
  $\mu_{k+1} = \mu_k + \triangle \mu$
end

where $\dot{T}$, $\dot{U}$, $\dot{A}$, $\dot{B}$ denote the derivatives with respect to μ of T, U, A, B, respectively, and

$$\begin{aligned} r &= T(\mu)y + U(\mu)v, & \dot{r} &= \dot{T}(\mu)y + \dot{U}(\mu)v, \\ s &= A(\mu)y + B(\mu)v, & \dot{s} &= \dot{A}(\mu)y + \dot{B}(\mu)v. \end{aligned} \tag{24}$$

if both $\mu + \triangle\mu$ and σ are close to the target eigenvalue, the last summand on the left-hand side of (23) will be small. Neglecting it and combining the remainder with the orthogonality condition (22) finally yields the linear system

$$\begin{bmatrix} T(\sigma) & U(\sigma) & \dot{r} \\ A(\sigma) & B(\sigma) & \dot{s} \\ y^{\mathsf{H}} & v^{\mathsf{H}} & 0 \end{bmatrix} \begin{bmatrix} \triangle y \\ \triangle v \\ \triangle \mu \end{bmatrix} = - \begin{bmatrix} r \\ s \\ 0 \end{bmatrix} \tag{25}$$

for computing the desired update.

By iteratively correcting an initial guess, we obtain Algorithm 1 to solve the augmented nonlinear eigenvalue problem (15). Local convergence of this algorithm towards simple eigenpairs can be proven using standard results [30, Theorem 4.1] on the convergence of simplified Newton methods. If the shift σ is updated in every step with the current eigenvalue approximation, Algorithm 1 is equivalent to nonlinear inverse iteration [31]. However, unlike nonlinear inverse iteration, keeping the shift constant to save computational work does not lead to erratic convergence. The convergence behavior for multiple eigenvalues is harder to analyze; see [17, 36] for convergence analyses of related methods in the presence of multiple eigenvalues. It is, however, easily seen from Theorem 3.5 that any multiple eigenvalue of the augmented eigenvalue problem (15) is a multiple eigenvalue of the original eigenproblem (1) as well. Hence, the difficulties are not inherent to the deflation approach in Section 3.

Once the algorithm has found a solution, the current invariant pair (X, Λ) is expanded via (8). According to Lemma 3.1 and 3.3, the resulting pair $(\hat{X}, \hat{\Lambda})$ is invariant and minimal.

4.2 A Jacobi-Davidson-type algorithm

Instead of directly updating the current iterate as in the previous subsection, the correction computed from the linear system (25) can also be used to expand the search space in a Petrov-Galerkin projection framework for solving the augmented nonlinear eigenvalue problem (15).

Algorithm 2: Nonlinear Jacobi-Davidson algorithm with deflation.

Input: minimal invariant pair (X, Λ), initial approximation (y_0, v_0, μ_0), basis for initial search space $\left[\begin{smallmatrix} Y_0 \\ V_0 \end{smallmatrix}\right]$, basis for initial test space $\left[\begin{smallmatrix} W_{1,0} \\ W_{2,0} \end{smallmatrix}\right]$

Output: extended minimal invariant pair $(\hat{X}, \hat{\Lambda})$

determine minimality index ℓ of (X, Λ)
for $k = 0, 1, 2, \ldots$ **do**
  compute residual $\left[\begin{smallmatrix} r \\ s \end{smallmatrix}\right]$ and derivative of residual $\left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right]$ as defined in (24)
  if *residual norm below convergence threshold* **then** build $(\hat{X}, \hat{\Lambda})$ via (8), stop.
  (approximately) solve correction equation (26) for $\left[\begin{smallmatrix} \triangle y \\ \triangle v \end{smallmatrix}\right]$
  expand search space $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$ to $\left[\begin{smallmatrix} Y_{k+1} \\ V_{k+1} \end{smallmatrix}\right]$ as in (28)
  expand test space $\left[\begin{smallmatrix} W_{1,k} \\ W_{2,k} \end{smallmatrix}\right]$ to $\left[\begin{smallmatrix} W_{1,k+1} \\ W_{2,k+1} \end{smallmatrix}\right]$ as in (29)
  solve projected eigenvalue problem by contour integral method
  if *no eigenvalues found* **then**
    perform Newton update $\left[\begin{smallmatrix} y_{k+1} \\ v_{k+1} \end{smallmatrix}\right] = \left[\begin{smallmatrix} y_k \\ v_k \end{smallmatrix}\right] + \left[\begin{smallmatrix} \triangle y \\ \triangle v \end{smallmatrix}\right]$
    set $\mu_{k+1} = \mu_k$
  else
    choose eigenpair (u, μ) of projected problem with μ closest to μ_k
    set $\mu_{k+1} = \mu$, $\left[\begin{smallmatrix} y_{k+1} \\ v_{k+1} \end{smallmatrix}\right] = \left[\begin{smallmatrix} Y_{k+1} \\ V_{k+1} \end{smallmatrix}\right] u$
  end
end

In this case, we are only interested in the $\triangle y$- and $\triangle v$-components of the solution. Hence, we eliminate $\triangle\mu$ from the system as follows. First, we recast the system as

$$\begin{bmatrix} T(\sigma) & U(\sigma) \\ A(\sigma) & B(\sigma) \end{bmatrix} \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} = - \begin{bmatrix} r + \dot{r}\triangle\mu \\ s + \dot{s}\triangle\mu \end{bmatrix}, \qquad \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} \perp \begin{bmatrix} y \\ v \end{bmatrix}.$$

Next, we premultiply by the oblique projector $I - \left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right] w^{\mathsf{H}}$ with the vector $w \in \mathbb{C}^{n+m}$ chosen orthogonal to $\left[\begin{smallmatrix} r \\ s \end{smallmatrix}\right]$ and normalized such that $w^{\mathsf{H}} \left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right] = 1$. This gives

$$\left(I - \begin{bmatrix} \dot{r} \\ \dot{s} \end{bmatrix} w^{\mathsf{H}} \right) \begin{bmatrix} T(\sigma) & U(\sigma) \\ A(\sigma) & B(\sigma) \end{bmatrix} \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} = - \begin{bmatrix} r \\ s \end{bmatrix}, \qquad \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} \perp \begin{bmatrix} y \\ v \end{bmatrix}.$$

Because of the orthogonality condition, the last equation can also be written as

$$\left(I - \begin{bmatrix} \dot{r} \\ \dot{s} \end{bmatrix} w^{\mathsf{H}} \right) \begin{bmatrix} T(\sigma) & U(\sigma) \\ A(\sigma) & B(\sigma) \end{bmatrix} \left(I - \begin{bmatrix} y \\ v \end{bmatrix} \begin{bmatrix} y \\ v \end{bmatrix}^{\mathsf{H}} \right) \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} = - \begin{bmatrix} r \\ s \end{bmatrix}, \qquad \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} \perp \begin{bmatrix} y \\ v \end{bmatrix}, \tag{26}$$

assuming, w.l.o.g., $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right]^{\mathsf{H}} \left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right] = 1$. Equation (26) has the form of a Jacobi-Davidson correction equation, similar to the work in [40] but with more freedom in the choice of w.

An algorithm for the solution of the augmented nonlinear eigenvalue problem (15) based on (26) would proceed as follows. Suppose that $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right] \in \mathbb{C}^{(n+m)\times k}$ is a matrix having orthonormal columns, which span the current search space. The current eigenvector approximation $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right]$ is then given by $(\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right] u, \mu)$, where (u, μ) with $u^{\mathsf{H}} u = 1$ is an eigenpair of the projected nonlinear eigenproblem

$$\begin{bmatrix} W_{1,k} \\ W_{2,k} \end{bmatrix}^{\mathsf{H}} \begin{bmatrix} T(\mu) & U(\mu) \\ A(\mu) & B(\mu) \end{bmatrix} \begin{bmatrix} Y_k \\ V_k \end{bmatrix} u = 0 \tag{27}$$

for some matrix $\left[\begin{smallmatrix} W_{1,k} \\ W_{2,k} \end{smallmatrix}\right] \in \mathbb{C}^{(n+m)\times k}$ with orthonormal columns. The eigenpair of the projected problem should be selected such that μ is as close as possible to the target eigenvalue of (15). Now the correction equation (26) is solved for $\triangle y, \triangle v$ and $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$ is expanded to $\left[\begin{smallmatrix} Y_{k+1} \\ V_{k+1} \end{smallmatrix}\right]$ having orthonormal columns such that

$$\operatorname{span} \begin{bmatrix} Y_{k+1} \\ V_{k+1} \end{bmatrix} = \operatorname{span} \left\{ \begin{bmatrix} Y_k \\ V_k \end{bmatrix}, \begin{bmatrix} \triangle y \\ \triangle v \end{bmatrix} \right\}. \tag{28}$$

The entire procedure is repeated with $\left[\begin{smallmatrix} Y_{k+1} \\ V_{k+1} \end{smallmatrix}\right]$ in place of $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$ until the desired accuracy of the approximate eigenpair is reached. Afterwards, the computed (y, v, μ) is used to expand the current invariant pair via (8). As in the previous section, the shift σ may be updated periodically to speed up convergence or kept constant to save computational work.

The above framework is summarized in Algorithm 2. In the following, we comment on the details of a practical implementation.

4.2.1 Choice of search and test spaces

We initialize the search space $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$ with a normalized random vector. The test space $\left[\begin{smallmatrix} W_{1,k} \\ W_{2,k} \end{smallmatrix}\right]$ is initialized with a normalized version of $\left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right]$ computed in the first step of the algorithm and then expanded in every iteration to include the current residual. That is, $\left[\begin{smallmatrix} W_{1,k+1} \\ W_{2,k+1} \end{smallmatrix}\right]$ is chosen such that it has orthonormal columns and

$$\operatorname{span} \begin{bmatrix} W_{1,k+1} \\ W_{2,k+1} \end{bmatrix} = \operatorname{span} \left\{ \begin{bmatrix} W_{1,k} \\ W_{2,k} \end{bmatrix}, \begin{bmatrix} r \\ s \end{bmatrix} \right\}. \tag{29}$$

This strategy can be viewed as a generalization of the harmonic Rayleigh-Ritz extraction procedure [29], which is frequently used within the Jacobi-Davidson algorithm for linear eigenvalue problems [32, 33].

4.2.2 Solution of the projected eigenproblems

To solve the projected eigenproblems, we employ the contour integral method [6, 1] followed by a few steps of Newton-based iterative refinement. As contour we choose a circle with a prescribed radius around the current eigenvalue approximation. Especially during the first steps of the algorithm, it may happen that there are no eigenvalues of the projected eigenproblem inside the contour. In this event, we use the computed solution of the correction equation (26) to update the eigenvector approximation to $\left[\begin{smallmatrix} y+\triangle y \\ v+\triangle v \end{smallmatrix}\right]$ as in the Newton method from the previous section while leaving the eigenvalue approximation unchanged.

In principle, any other solution method for nonlinear eigenvalue problems could be used as well to handle the projected problems. Most notably, when dealing with polynomial eigenvalue problems, the augmented problem (15) will also be polynomial, facilitating the use of linearization techniques [12, 23]. Ideally, the method of choice should be able to benefit significantly from the small size of the projected problems.

4.2.3 Solution of the correction equation

As is typical for a Jacobi-Davidson iteration, the correction equation (26) need not be solved very accurately. A few steps of a preconditioned Krylov subspace method, such as GMRES, are usually enough. In our experiments, we have tested stopping the Krylov solver after having

decreased the residual by a prescribed factor as well as stopping the solver after a fixed number of iterations. Both strategies seem to work equally well.

To enable the iterative solution of the correction equation (26), we are in need of an effective preconditioner. In the following, we will describe how a suitable preconditioner can be constructed, given a preconditioner for $T(\mu)$. Devising a good preconditioner for $T(\mu)$ is a highly application-dependent task and therefore beyond the scope of this article.

Recalling that the blocks within the matrix

$$\mathcal{T} = \begin{bmatrix} T & U \\ A & B \end{bmatrix} \tag{30}$$

associated with the augmented nonlinear eigenvalue problem (15) have different origins, it seems wise to take the block structure into account when thinking about preconditioning. Note that we have dropped the explicit dependence on μ here for the sake of better readability. A rich theory on preconditioning of 2×2 block systems is available in the literature; see [3] and the references therein. Unfortunately, most of the existing methods require the blocks to possess additional properties, such as symmetry or definiteness, which, in general, are not present in $\mathcal{T}$. For this reason, we will pursue a different approach.

Consider the block triangular factorization

$$\begin{bmatrix} T & U \\ A & B \end{bmatrix} = \begin{bmatrix} I & 0 \\ AT^{-1} & I \end{bmatrix} \begin{bmatrix} T & U \\ 0 & B - AT^{-1}U \end{bmatrix}$$

of $\mathcal{T}$. The inverse of the right block triangular factor reads

$$\begin{bmatrix} T^{-1} & -T^{-1}U(B - AT^{-1}U)^{-1} \\ 0 & (B - AT^{-1}U)^{-1} \end{bmatrix}.$$

Approximating, the upper, left block of this inverse by a given preconditioner P^{-1} for T, yields the matrix

$$\mathcal{P}^{-1} = \begin{bmatrix} P^{-1} & -T^{-1}U(B - AT^{-1}U)^{-1} \\ 0 & (B - AT^{-1}U)^{-1} \end{bmatrix}, \tag{31}$$

which we will employ as a preconditioner for $\mathcal{T}$.

Proposition 4.1. *Assume that the matrix $\mathcal{T}$ in (30) is preconditioned by $\mathcal{P}$ as in (31). Then the spectrum of the preconditioned matrix $\mathcal{T}\mathcal{P}^{-1}$ consists of the spectrum of TP^{-1} and the eigenvalue 1. Furthermore, the degree of the minimal polynomial of $\mathcal{T}\mathcal{P}^{-1}$ exceeds the degree of the minimal polynomial of TP^{-1} by at most one.*

Proof. The statement about the spectrum is obvious from the structure of the preconditioned matrix,

$$\mathcal{T}\mathcal{P}^{-1} = \begin{bmatrix} TP^{-1} & 0 \\ AP^{-1} & I \end{bmatrix}.$$

For the second statement, let p be the minimal polynomial of TP^{-1}. One easily calculates that $(\mathcal{T}\mathcal{P}^{-1} - I) \cdot p(\mathcal{T}\mathcal{P}^{-1}) = 0$. Consequently, the minimal polynomial of $\mathcal{T}\mathcal{P}^{-1}$ must be a divisor of $(\lambda - 1) \cdot p(\lambda)$, implying the claimed bound on its degree. □

Proposition 4.1 shows that the preconditioner $\mathcal{P}^{-1}$ for $\mathcal{T}$ has about the same quality as the preconditioner P^{-1} for T from which it has been constructed. However, it may seem that one needs to know T^{-1} in order to apply $\mathcal{P}^{-1}$. To eliminate this flaw, we utilize the subsequent lemma.

Lemma 4.2. *Let (X, Λ) be an invariant pair of the nonlinear eigenvalue problem (1) and let U be defined as in 10. Then for any $\mu \in \Omega$,*

$$U(\mu)(\mu I - \Lambda) = T(\mu)X.$$

Proof. A direct calculation using $\mu I - \Lambda = (zI - \Lambda) - (z - \mu)I$ shows

$$\begin{aligned} U(\mu)(\mu I - \Lambda) &= \frac{1}{2\pi \mathrm{i}} \int_\Gamma T(z)X(z-\mu)^{-1}\,\mathrm{d}z - \frac{1}{2\pi \mathrm{i}} \int_\Gamma T(z)X(zI-\Lambda)^{-1}\,\mathrm{d}z \\ &= T(\mu)X - \mathbf{T}(X, \Lambda). \end{aligned}$$

The proof is finished by concluding from Definition 2.1 that $\mathbf{T}(X, \Lambda) = 0$. □

Suppose that μ is not an eigenvalue of T. Note that this also implies that μ is not an eigenvalue of Λ if the pair (X, Λ) is minimal invariant. Then Lemma 4.2 implies $T(\mu)^{-1}U(\mu) = X(\mu I - \Lambda)^{-1}$. However, if μ is close to an eigenvalue of Λ, the matrix $\mu I - \Lambda$ might be arbitrarily ill-conditioned. We therefore utilize $T(\mu)^{-1}U(\mu) = X(\mu I - \Lambda)^\dagger$ instead. The size of the matrix $\mu I - \Lambda$ can be expected to be rather small, so the Moore-Penrose pseudoinverse $(\mu I - \Lambda)^\dagger$ is efficiently computable by means of the singular value decomposition. Thus, the preconditioner applied in practice reads

$$\tilde{\mathcal{P}}^{-1} = \begin{bmatrix} P^{-1} & -X(\mu I - \Lambda)^\dagger \big(B - AX(\mu I - \Lambda)^\dagger\big)^{-1} \\ 0 & \big(B - AX(\mu I - \Lambda)^\dagger\big)^{-1} \end{bmatrix}.$$

Its application to a vector requires one linear system solve with P and the Schur complement $B - AX(\mu I - \Lambda)^\dagger$ each as well as one matrix-vector multiplication by $X(\mu I - \Lambda)^\dagger$. Since the Schur complement is as small as the matrix $\mu I - \Lambda$, it can be inverted by a direct solver at negligible cost. Consequently, the computational work for applying $\tilde{\mathcal{P}}^{-1}$ is essentially that of applying P^{-1}.

In the Jacobi-Davidson correction equation (26), the matrix $\mathcal{T}$ is surrounded by projectors, which restrict its action to a map from the orthogonal complement of $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right]$ to the orthogonal complement of w. The same restriction should be applied to the preconditioner [33, 40]. It is straightforward to compute that the appropriately projected preconditioner is given by

$$\left(I - \frac{\tilde{\mathcal{P}}^{-1}\left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right]\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right]^{\mathsf{H}}}{\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right]^{\mathsf{H}}\tilde{\mathcal{P}}^{-1}\left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right]}\right)\tilde{\mathcal{P}}.$$

Every application of the projector costs just one inner product. Additionally, we have to apply the preconditioner $\tilde{\mathcal{P}}^{-1}$ to $\left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right]$ and take the inner product with $\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right]$ once in a preprocessing step.

4.2.4 Evaluating the residuals and projected problems

In every step of Algorithm 2, we have to evaluate the residual $\left[\begin{smallmatrix} r \\ s \end{smallmatrix}\right]$ and its derivative $\left[\begin{smallmatrix} \dot{r} \\ \dot{s} \end{smallmatrix}\right]$ as defined in (24). A similar calculation as in the proof of Lemma 3.1 shows that r and $\dot{r}$ can be computed at once from the block residual $\mathbf{T}\Big(\big[X, y, 0\big], \left[\begin{smallmatrix} \Lambda & v & \\ & \mu & 1 \\ & & \mu \end{smallmatrix}\right]\Big) = \big[\mathbf{T}(X, \Lambda), r, \dot{r}\big]$ of the original nonlinear eigenproblem (1). From the definitions of $A(\mu)$ and $B(\mu)$ in (14), it is evident that evaluating s and $\dot{s}$ involves mainly operations on small matrices and vectors,

the only exceptions being the computation of $X^{\mathsf{H}}y$ and $X^{\mathsf{H}}X$. The latter, however, can be precomputed incrementally as X is built up. Using the calculus of matrix functions [14], the necessary polynomial evaluations can be conveniently combined into computing the matrix polynomials $p_i\Big(\begin{bmatrix} \Lambda & v \\ & \mu & 1 \\ & & \mu \end{bmatrix}\Big) = \begin{bmatrix} p_i(\Lambda) & q_i(\mu)v & \dot{q}_i(\mu)v \\ & p_i(\mu) & \dot{p}_i(\mu) \\ & & p_i(\mu) \end{bmatrix}$, $i = 0, \ldots, \ell$.

The evaluation of the matrices associated with the projected nonlinear eigenproblems (27) proceeds in a similar fashion as above. If the block residual admits a representation of the form (4), the computational effort can be reduced by working with the projected coefficient matrices $W_{1,k}^{\mathsf{H}} T_j\big[X, Y_k\big]$, $j = 1, \ldots, d$. Again, it is beneficial to incrementally build up these projected coefficient matrices as we expand X or the search and test spaces.

4.2.5 Restarting, Locking and Purging

The Jacobi-Davidson algorithm 2 is designed to aim at one eigenpair at a time. However, the search space may also contain approximations to eigenvectors whose corresponding eigenvalue lies close to the current target and it is desirable to use this information. On the other hand, we must not let the search space grow too large due to memory constraints. To keep the size of the search space at a moderate level, it needs to be purged periodically, i.e., replaced by a subspace of smaller dimension, which (hopefully) still contains the most valuable information. Since purging impedes convergence, we purge the search space only immediately after a target eigenpair has converged.

Assume that convergence occurs at the k-th step of Algorithm 2. If the current search space $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$ contains sufficient information about further eigenpairs, approximations to these eigenpairs will show up as solutions of the projected nonlinear eigenvalue problem (27). These approximations will be discovered by the contour integral method used to solve (27), provided that the associated eigenvalues lie close enough to the target. We will thus obtain a minimal invariant pair (C, M) of the projected eigenproblem (27), representing all eigenvalues inside the contour. By lifting this pair to the full space, $\big(\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right] C, M\big)$ is an approximate minimal invariant pair of the augmented nonlinear eigenvalue problem (15). Hence, in compressing the search space to the range of $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right] C$, we retain only the information necessary to reproduce the eigenpairs encoded by (C, M). If (C, M) consists only of the target eigenpair, we take this as an indication that no more relevant information is present in $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$. In this case, the search space is purged entirely and replaced by a normalized, random vector unless further targets are left from previous restarts. Likewise, the contour integral method supplies information about the left eigenvectors, which can be used analogously to compress the test space $\left[\begin{smallmatrix} W_{1,k} \\ W_{2,k} \end{smallmatrix}\right]$.

Unfortunately, we cannot simply continue Algorithm 2 with the compressed search and test spaces because locking the currently converged eigenpair via (8) will increase the dimension of the augmented nonlinear eigenproblem (15) by one. Consequently, the search and test spaces need to be adjusted accordingly. We begin by describing this adjustment for the search space. W.l.o.g., we can assume M to be in Schur form, ordered in such a way that the first diagonal entry of M is the target eigenvalue and the second diagonal entry is the eigenvalue approximation we would like to select as the next target. Otherwise, we compute a unitary matrix Q such that $Q^{\mathsf{H}}MQ$ has the desired form and work with the pair $(CQ, Q^{\mathsf{H}}MQ)$ instead; compare Lemma 2.5. Partitioning

$$\begin{bmatrix} Y_k \\ V_k \end{bmatrix} C = \begin{bmatrix} y_1 & Y_2 \\ v_1 & V_2 \end{bmatrix}, \qquad M = \begin{bmatrix} \mu & m_{12} \\ 0 & M_{22} \end{bmatrix}$$

such that $y_1 \in \mathbb{C}^n$ and $v_1 \in \mathbb{C}^m$ are vectors and μ is a scalar, $(\left[\begin{smallmatrix} y_1 \\ v_1 \end{smallmatrix}\right], \mu)$ is the eigenpair of the augmented eigenproblem (15) which is going to be locked. If $(\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right] C, M)$ was an exact minimal invariant pair of the augmented problem (15), then by Theorem 3.5,

$$\left(\begin{bmatrix} X & y_1 & Y_2 \end{bmatrix}, \begin{bmatrix} \Lambda & v_1 & V_2 \\ 0 & \mu & m_{12} \\ 0 & 0 & M_{22} \end{bmatrix} \right)$$

would be a minimal invariant pair of the original nonlinear eigenvalue problem (1). Locking the eigenpair $\left(\left[\begin{smallmatrix} y_1 \\ v_1 \end{smallmatrix}\right], \mu\right)$ and applying Theorem 3.5 again, we find that for a suitably chosen matrix F,

$$\left(\begin{bmatrix} Y_2 - \begin{bmatrix} X & y_1 \end{bmatrix} F \\ \begin{bmatrix} V_2 \\ m_{12} \end{bmatrix} - \left(\begin{bmatrix} \Lambda & v_1 \\ 0 & \mu \end{bmatrix} F - F M_{22} \right) \end{bmatrix}, M_{22} \right)$$

is a minimal invariant pair of the new augmented eigenproblem (15). Recall from the proof of Theorem 3.5 that the choice of F only influences the minimality constraint (13) but neither the invariance constraint (9) nor the minimality of the ensuing pair itself. Moreover, we have not observed a significant gain be choosing the correct F in our experiments. Therefore, we save some computational work by setting $F = 0$. Performing an economy-size QR decomposition, $\left[\begin{smallmatrix} Y_2 \\ V_2 \\ m_{12} \end{smallmatrix}\right] = QR$, the resulting pair is transformed to $(Q, RM_{22}R^{-1})$ according to Lemma 2.5. We then take Q as basis for the new search space and the first diagonal element of $RM_{22}R^{-1}$ as the new shift. If $(Q, RM_{22}R^{-1})$ contains more than one eigenpair, the unused ones are stored for future restarts.

Transforming the test space in a similar way does not make sense because the minimality conditions (13) before and after the locking are very different. Instead we propose partitioning the compressed test space as $\left[\begin{smallmatrix} W_1 \\ W_2 \end{smallmatrix}\right]$ conformally with the block structure of the augmented nonlinear eigenvalue problem (15) and then taking the new test space as the range of $\left[\begin{smallmatrix} W_1 \\ 0 \end{smallmatrix}\right]$.

4.2.6 Selective deflation

The computational effort per iteration of Algorithm 2 grows with the number of columns, m, inside the deflated minimal invariant pair $(X, \Lambda) \in \mathbb{C}^{n \times m} \times \mathbb{C}^{m \times m}$. This effect, however, becomes severe only for large values of m. More dramatically, a larger invariant pair might have a higher minimality index, which is already indicated by the fact that the minimality index is bounded by m [20, Lemma 5].

A higher minimality index impacts the evaluation of $A(\mu)$ and $B(\mu)$ defined in (14) in two ways. Firstly, it increases the necessary computational work by increasing the number of summands in (14). Besides and more importantly, it complicates the selection of a polynomial basis $p_0, \ldots, p_\ell$ which avoids numerical instabilities in forming $A(\mu)$, $B(\mu)$ if the eigenvalues of Λ are not very well clustered; see the discussion in Section 2.

It is therefore desirable to keep the size of the deflated minimal invariant pair as small as possible. The key to doing so lies in the observation that since Algorithm 2 operates only locally, reconvergence can only occur for eigenvalues which are close to the current target μ_0. In particular, if we solve the projected eigenproblems (27) by the contour integral method, where the contour is a circle of radius ρ around μ_0, only eigenvalues λ satisfying $|\lambda - \mu_0| \leq \rho$ are threatened by reconvergence. This motivates the following approach. We reorder (X, Λ)

by a unitary transformation Q into an equivalent (in the sense of Lemma 2.5) pair

$$(XQ, Q^{\mathsf{H}}\Lambda Q) = \left(\begin{bmatrix} X_1 & X_2 \end{bmatrix}, \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ & \Lambda_{22} \end{bmatrix} \right) \tag{32}$$

such that the eigenvalues of Λ_{11} and Λ_{22} lie inside and outside of the ball with radius $\gamma \cdot \rho$ around the target μ, respectively. Here, $\gamma > 1$ is a safety factor intended to compensate for possible updates of the target μ within the course of the algorithm. The search and test spaces $\left[\begin{smallmatrix} Y_k \\ V_k \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} W_{1,k} \\ W_{2,k} \end{smallmatrix}\right]$ have to be transformed accordingly to $\left[\begin{smallmatrix} Y_k \\ Q^{\mathsf{H}} V_k \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} W_{1,k} \\ Q^{\mathsf{H}} W_{2,k} \end{smallmatrix}\right]$, respectively. We then construct the augmented nonlinear eigenvalue problem (15) only from (X_1, Λ_{11}). Since (X_1, Λ_{11}) tends to have fewer columns than the full pair (X, Λ), we have achieved our goal. Moreover, the eigenvalues of Λ_{11} are contained inside a ball. Thus, they tend to be better clustered than those of Λ, simplifying the choice of an appropriate polynomial basis.

While running Algorithm 2 to solve the augmented eigenproblem (15), we carefully monitor whether the eigenvalue approximation moves close to an eigenvalue of Λ_{22}, and if so, adjust the partitioning (32). This ensures that the algorithm computes an eigenpair $\left(\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right], \mu\right)$ such that μ is not within the spectrum of Λ_{22}. In lieu of the classical update (8), we then perform the expansion $(\hat{X}, \hat{\Lambda}) = \left(\begin{bmatrix} X_1, X_2, y \end{bmatrix}, \left[\begin{smallmatrix} \Lambda_{11} & \Lambda_{12} & v \\ & \Lambda_{22} & 0 \\ & & \mu \end{smallmatrix}\right] \right)$, which is justified by the subsequent lemma.

Lemma 4.3. *Let* $\left([X_1, X_2], \left[\begin{smallmatrix} \Lambda_{11} & \Lambda_{12} \\ & \Lambda_{22} \end{smallmatrix}\right]\right)$ *and* $\left([X_1, Y], \left[\begin{smallmatrix} \Lambda_{11} & V \\ & M \end{smallmatrix}\right]\right)$ *be minimal invariant pairs of the nonlinear eigenproblem* (1) *and assume that* Λ_{22} *and* M *have no eigenvalues in common. Then the extended pair* $\left([X_1, X_2, Y], \left[\begin{smallmatrix} \Lambda_{11} & \Lambda_{12} & V \\ & \Lambda_{22} & 0 \\ & & M \end{smallmatrix}\right]\right)$ *is minimal and invariant.*

Proof. The invariance follows by expanding and comparing the block residuals of the three pairs as in the proof of Lemma 3.1. To prove the minimality, we have to show that the equation

$$\begin{bmatrix} X_1 & X_2 & Y \\ \Lambda_{11} - \lambda I & \Lambda_{12} & V \\ & \Lambda_{22} - \lambda I & 0 \\ & & M - \lambda I \end{bmatrix} \begin{bmatrix} g_1 \\ g_2 \\ h \end{bmatrix} = 0$$

admits only the zero solution. Since Λ_{22} and M do not have any eigenvalues in common, at least one of the matrices $\Lambda_{22} - \lambda I$, $M - \Lambda I$ is invertible. W.l.o.g., assume the latter is invertible; otherwise, similar arguments apply. Then the last block row of the equation implies $h = 0$, leaving us with $\left[\begin{smallmatrix} X_1 & X_2 \\ \Lambda_{11} - \lambda I & \Lambda_{12} \\ & \Lambda_{22} - \lambda I \end{smallmatrix}\right] \left[\begin{smallmatrix} g_1 \\ g_2 \end{smallmatrix}\right] = 0$, which only admits the zero solution thanks to the minimality of the first pair. □

Because Lemma 4.3 applies to blocks $\left(\left[\begin{smallmatrix} Y \\ V \end{smallmatrix}\right], M\right)$ and not just eigenpairs $\left(\left[\begin{smallmatrix} y \\ v \end{smallmatrix}\right], \mu\right)$, the restarting mechanism from Section 4.2.5 remains valid in the case of selective deflation.

5 Numerical experiments

To demonstrate the effectiveness of our approach, we apply a MATLAB implementation of Algorithm 2 to several test problems. All computations are run under MATLAB 7.13 (R2011b) on an Intel® Core™ i7-2640M processor with 2.8 GHz and 4 GB of memory. The presented residuals are computed by $\frac{\|T(\mu)y + U(\mu)v\|_2}{\|T(\mu)\|_{\mathsf{F}}}$ with U defined as in (10) and $\|\cdot\|_{\mathsf{F}}$ denoting the Frobenius norm.

Our implementation always solves the projected problems by the contour integral method, even for the last experiment, where the problem at hand is polynomial and hence eligible for

linearization. The contours are circles around the current eigenvalue approximations, whose radius ρ depends on the problem. We employ the selective deflation strategy from Section 4.2.6 with safety factor $\gamma = 1.2$ and restart the algorithm as outlined in Section 4.2.5. For the deflation, we use the polynomial basis $p_i(\lambda) = \alpha^i(\lambda - \mu)^i$, where μ is the current target and $\alpha = (\gamma\rho)^{-1}$.

The correction equations are solved iteratively by GMRES. The solver is stopped after at most 10 iterations or earlier if the residual has been decreased by a factor of 10^{-2}. The shift σ is updated in every step with the current eigenvalue approximation.

In every experiment, we start the Jacobi-Davidson algorithm using certain approximations to the desired eigenvalues. How these approximations are obtained is described within the individual subsections. The starting vectors, however, are always picked at random and we do not inject any knowledge about the eigenvectors.

5.1 Delay eigenvalue problem

As our first experiment, we consider the parabolic partial differential equation

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) + a_0 u(x,t) + a_1(x)u(x,t-\tau), \qquad u(0,t) = u(\pi,t) = 0 \tag{33}$$

with time delay τ and coefficients $a_0 = 20$, $a_1(x) = -4.1 + x(1 - \mathrm{e}^{x-\pi})$, taken from [15, Sec. 2.4.1], which is a modification of [41, Chapter 3, Example 1.12]. Discretizing (33) in space by finite differences on the uniform grid $\{x_i = \frac{i}{n+1}\pi : i = 1, \ldots, n\}$ of size $h = \frac{\pi}{n+1}$ leads to the delay differential equation

$$\dot{v}(t) = A_0 v(t) + A_1 v(t-\tau) \tag{34}$$

with the coefficient matrices $A_0 = \left(\frac{\pi}{n+1}\right)^2 \begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix} + a_0 I$, $A_1 = \begin{bmatrix} a_1(x_1) & & \\ & \ddots & \\ & & a_1(x_n) \end{bmatrix} \in \mathbb{R}^{n\times n}$ and $v(t) = \big[u(x_1,t), \ldots, u(x_n,t)\big]^{\mathsf{T}}$. An asymptotic stability analysis of (34) requires a few largest real part eigenvalues of the delay eigenvalue problem $T(\lambda)v = 0$ with

$$T(\lambda) = -\lambda I + A_0 + \mathrm{e}^{-\tau\lambda} A_1.$$

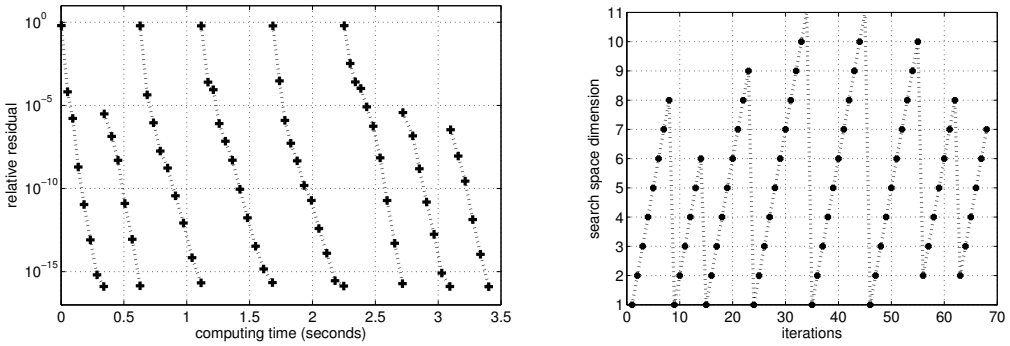

Figure 1: Left. Convergence history for the delay eigenvalue problem. Right. Evolution of the search space dimension.

For our experiment, we choose $n = 1000$, $\tau = 0.2$. As a preconditioner for $T(\lambda)$, we employ the discrete second derivative $P = \left(\frac{\pi}{n+1}\right)^2 \begin{bmatrix} -2 & 1 & & \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{bmatrix}$. Note that $-P$ is positive definite and can thus be efficiently inverted via a sparse Cholesky decomposition. If λ has a large, positive real part, $\mathrm{e}^{-\tau\lambda}$ tends to be small, implying $T(\lambda) \approx A_0 - \lambda I$. This encourages using the eigenvalues of A_0 with largest real part as starting values.

The left plot in Figure 1 illustrates the convergence of the 8 largest real eigenvalues of T. The eigenvalues computed are in this order: 18.932251, 15.868175, 10.618574, 1.733673, -5.342532, -9.215977, -10.717667, -11.818305. The computations of the 2^{nd}, 7^{th}, and 8^{th} eigenvalue have been warm-started using the restarting technique from Section 4.2.5. As a result, their initial residuals are considerably lower than those of the other eigenvalues, where no information could be reused from the previous run. The evolution of the search space is depicted on the right in Figure 1; its dimension never exceeds 11.

5.2 Radio-frequency gun cavity

As a second example, we consider

$$T(\lambda) = K - \lambda M + \mathrm{i}\sqrt{\lambda^2 - \sigma_1^2}\, W_1 + \mathrm{i}\sqrt{\lambda^2 - \sigma_2^2}\, W_2,$$

taken from [4]. It models a radio-frequency gun cavity; for details, see also [22]. $\sqrt{\cdot}$ denotes the principal branch of the complex square root. The matrices $K, M, W_1, W_2 \in \mathbb{R}^{9956\times 9956}$ are

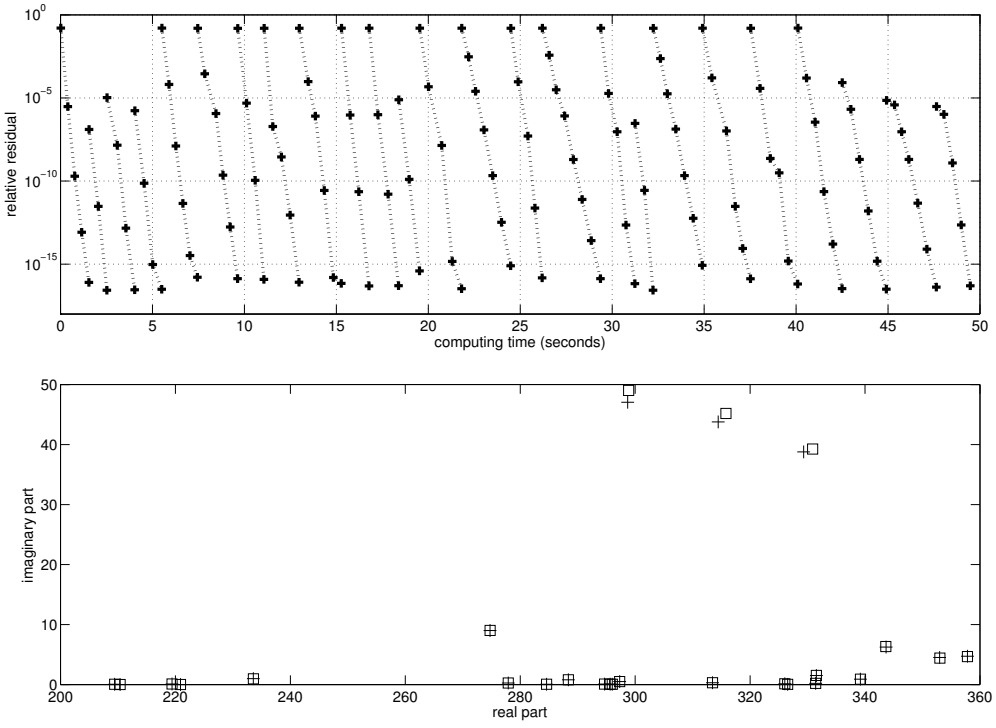

Figure 2: Top. Convergence history for the gun example. Bottom. Eigenvalues computed by Algorithm 2 (+) and approximate eigenvalues from linearized problem (□).

symmetric and sparse, $\sigma_1 = 0$, and $\sigma_2 = 108.8774$. Linearizing the square roots around $\lambda_0^2 - \sigma_i^2$, we find

$$T(\lambda) \approx \left(K + \tfrac{\mathrm{i}(\lambda_0^2 - 2\sigma_1^2)}{2\sqrt{\lambda_0^2 - \sigma_1^2}} W_1 + \tfrac{\mathrm{i}(\lambda_0^2 - 2\sigma_2^2)}{2\sqrt{\lambda_0^2 - \sigma_2^2}} W_2\right) - \lambda^2 \left(M - \tfrac{\mathrm{i}}{2\sqrt{\lambda_0^2 - \sigma_1^2}} W_1 - \tfrac{\mathrm{i}}{2\sqrt{\lambda_0^2 - \sigma_2^2}} W_2\right),$$

which is linear in λ^2 and provides excellent approximations to eigenvalues close to λ_0.

For our, experiment, we take $\lambda_0^2 = 81250$ and aim at computing the 25 eigenvalues of T closest to λ_0. The bottom part of Figure 2 displays the computed eigenvalues (+) along with the approximations (□) from the linearized problem above. The abundance of tightly clustered eigenvalues in this example is particularly appealing for testing our algorithm, which exhibits no flaws in determining them correctly. The convergence history is presented in the top part of Figure 2. The merits of our restarting procedure are again clearly visible for eigenvalues number 2, 3, 4, 12, 18, 23, 24, 25.

5.3 Boundary element discretization of Laplace eigenvalue problem

As our final example, we consider a polynomial interpolant $T(\lambda) = \tau_0(\lambda)P_0 + \cdots + \tau_d(\lambda)P_d$ of a matrix-valued function stemming from a boundary element discretization of the Laplace eigenvalue problem with Dirichlet boundary conditions on the unit cube; see [34, 9]. For stability reasons, the polynomial is given in the Chebyshev basis $\tau_0, \ldots, \tau_d$. The coefficient matrices are complex of order 2400×2400.

We are interested in computing the six smallest eigenvalues of T. In the continuous setting, the multiplicities of these eigenvalues are 1, 3, 3, 3, 1, 6. As a result, the polynomial T has very tight eigenvalue clusters, agreeing up to 10 decimal places, making it very hard for a Newton-based method. In consequence, we observe some non-monotonic convergence behavior in Figure 3. However, the algorithm does retrieve the correct number of eigenvalues in each cluster. Moreover, after the first eigenvalue in a cluster has converged, our restarting strategy helps to find the remaining ones more quickly. This is especially apparent from the six-fold eigenvalue, which has been computed first.

Conclusion

We have presented a technique to deflate arbitrary minimal invariant pairs from a given nonlinear eigenvalue problem. This greatly enhances the performance of Newton-based methods

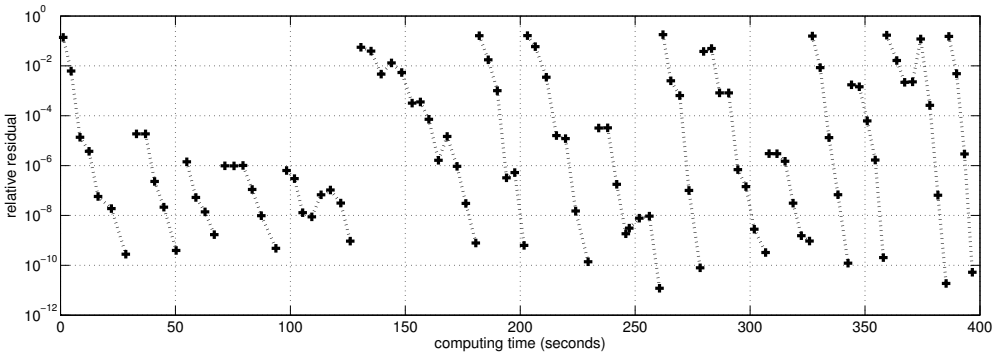

Figure 3: Convergence history for the boundary element example.

by eliminating their tendency to reconverge to previously determined eigenpairs. The deflation takes place via a suitable bordering of the original nonlinear eigenvalue problem, leading to a problem of slightly increased size.

We have incorporated this deflation technique into a Jacobi-Davidson-type algorithm. Various algorithmic details have been discussed, including a restarting strategy capable of handling the increase in problem size as additional eigenpairs are locked. By employing a suitable preconditioner for the correction equation and selectively deflating only specific eigenpairs, the computational overhead incurred by the deflation is kept to a minimum.

The effectiveness of the ensuing algorithm has been demonstrated by means of several numerical experiments. Moreover, it should be emphasized that the algorithm only requires the block residual and a preconditioner for the original nonlinear eigenvalue problem to run. Thus, it is qualified for implementation as a black-box solver.

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References

[1] J. Asakura, T. Sakurai, H. Tadano, T. Ikegami, and K. Kimura. A numerical method for nonlinear eigenvalue problems using contour integrals. *JSIAM Letters*, 1:52–55, 2009.

[2] Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst, editors. *Templates for the solution of Algebraic Eigenvalue Problems: A Practical Guide*. SIAM, Philadelphia, 2000.

[3] M. Benzi, G. H. Golub, and J. Liesen. Numerical solution of saddle point problems. *Acta Numer.*, 14:1–137, 2005.

[4] T. Betcke, N. J. Higham, V. Mehrmann, C. Schröder, and F. Tisseur. NLEVP: A collection of nonlinear eigenvalue problems. MIMS EPrint 2011.116, Manchester Institute for Mathematical Sciences, The University of Manchester, UK, Dec. 2011.

[5] T. Betcke and L. N. Trefethen. Reviving the method of particular solutions. *SIAM Rev.*, 47(3):469–491, 2005.

[6] W.-J. Beyn. An integral method for solving nonlinear eigenvalue problems. *Linear Algebra and its Applications*, 436(10):3839–3863, 2012.

[7] W.-J. Beyn, C. Effenberger, and D. Kressner. Continuation of eigenvalues and invariant pairs for parameterized nonlinear eigenvalue problems. *Numer. Math.*, 119(3):489–516, 2011.

[8] M. A. Botchev, G. L. G. Sleijpen, and A. Sopaheluwakan. An SVD-approach to Jacobi-Davidson solution of nonlinear Helmholtz eigenvalue problems. *Linear Algebra Appl.*, 431(3-4):427–440, 2009.

[9] C. Effenberger and D. Kressner. Chebyshev interpolation for nonlinear eigenvalue problems. *BIT Numerical Mathematics*, 2012. To appear. DOI: 10.1007/s10543-012-0381-5.

[10] C. Engström and M. Wang. Complex dispersion relation calculations with the symmetric interior penalty method. *Internat. J. Numer. Methods Engrg.*, 84(7):849–863, 2010.

[11] D. R. Fokkema, G. L. G. Sleijpen, and H. A. Van der Vorst. Jacobi-Davidson style QR and QZ algorithms for the reduction of matrix pencils. *SIAM J. Sci. Comput.*, 20(1):94–125, 1998.

[12] I. Gohberg, P. Lancaster, and L. Rodman. *Matrix polynomials*. Academic Press, New York, 1982. Computer Science and Applied Mathematics.

[13] M. L. J. Hautus. Controllability and observability conditions of linear autonomous systems. *Nederl. Akad. Wetensch. Proc. Ser. A 72 = Indag. Math.*, 31:443–448, 1969.

[14] N. J. Higham. *Functions of matrices*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2008.

[15] E. Jarlebring. *The spectrum of delay-differential equations: numerical methods, stability and perturbation*. PhD thesis, Inst. Comp. Math, TU Braunschweig, 2008.

[16] E. Jarlebring, K. Meerbergen, and W. Michiels. Computing a partial schur factorization of nonlinear eigenvalue problems using the infinite arnoldi method. Technical report, Dept. Comp. Science, K.U. Leuven, 2011.

[17] E. Jarlebring and W. Michiels. Analyzing the convergence factor of residual inverse iteration. *BIT*, 51(4):937–957, 2011.

[18] E. Jarlebring, W. Michiels, and K. Meerbergen. A linear eigenvalue algorithm for the nonlinear eigenvalue problem. *Numerische Mathematik*, 2012. To appear.

[19] N. Kamiya and S. T. Wu. Generalized eigenvalue formulation of the Helmholtz equation by the Trefftz method. *Engineering Computations*, 11:177–186, 1994.

[20] D. Kressner. A block Newton method for nonlinear eigenvalue problems. *Numer. Math.*, 114(2):355–372, 2009.

[21] R. B. Lehoucq and D. C. Sorensen. Deflation techniques for an implicitly restarted Arnoldi iteration. *SIAM J. Matrix Anal. Appl.*, 17(4):789–821, 1996.

[22] B.-S. Liao, Z. Bai, L.-Q. Lee, and K. Ko. Nonlinear Rayleigh-Ritz iterative method for solving large scale nonlinear eigenvalue problems. *Taiwanese J. Math.*, 14(3A):869–883, 2010.

[23] D. S. Mackey, N. Mackey, C. Mehl, and V. Mehrmann. Vector spaces of linearizations for matrix polynomials. *SIAM J. Matrix Anal. Appl.*, 28(4):971–1004, 2006.

[24] Karl Meerbergen. Locking and restarting quadratic eigenvalue solvers. *SIAM J. Sci. Comput.*, 22(5):1814–1839, 2000.

[25] V. Mehrmann and H. Voss. Nonlinear eigenvalue problems: A challenge for modern eigenvalue methods. *GAMM Mitt. Ges. Angew. Math. Mech.*, 27(2):121–152, 2004.

[26] R. Mennicken and M. Möller. *Non-self-adjoint boundary eigenvalue problems*, volume 192 of *North-Holland Mathematics Studies*. North-Holland Publishing Co., Amsterdam, 2003.

[27] W. Michiels and S.-I. Niculescu. *Stability and stabilization of time-delay systems. An eigenvalue-based approach*, volume 12 of *Advances in Design and Control*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2007.

[28] E. Moreno, D. Erni, and C. Hafner. Band structure computations of metallic photonic crystals with the multiple multipole method. *Phys. Rev. B*, 65(15):155120–1–155120–10, Apr. 2002.

[29] C. C. Paige, B. N. Parlett, and H. A. van der Vorst. Approximate solutions and eigenvalue bounds from Krylov subspaces. *Numer. Linear Algebra Appl.*, 2(2):115–133, 1995.

[30] W. C. Rheinboldt. A unified convergence theory for a class of iterative processes. *SIAM J. Numer. Anal.*, 5:42–63, 1968.

[31] A. Ruhe. Algorithms for the nonlinear eigenvalue problem. *SIAM J. Numer. Anal.*, 10:674–689, 1973.

[32] G. L. G. Sleijpen and H. A. Van der Vorst. A Jacobi-Davidson iteration method for linear eigenvalue problems. *SIAM Rev.*, 42(2):267–293, 2000.

[33] G. L. G. Sleijpen, H. A. van der Vorst, and E. Meijerink. Efficient expansion of subspaces in the Jacobi-Davidson method for standard and generalized eigenproblems. *Electron. Trans. Numer. Anal.*, 7:75–89, 1998.

[34] O. Steinbach and G. Unger. A boundary element method for the Dirichlet eigenvalue problem of the Laplace operator. *Numer. Math.*, 113(2):281–298, 2009.

[35] G. W. Stewart. A Krylov-Schur algorithm for large eigenproblems. *SIAM J. Matrix Anal. Appl.*, 23(3):601–614, 2001/02.

[36] G. Unger. Convergence orders of iterative methods for nonlinear eigenvalue problems. In T. Apel and O. Steinbach, editors, *Advanced Finite Element Methods and Applications*, volume 66 of *Lecture Notes of Applied and Computational Mechanics*, pages 217–238. Springer, New York, 2012.

[37] H. Voss. A rational spectral problem in fluid-solid vibration. *Electron. Trans. Numer. Anal.*, 16:93–105, 2003.

[38] H. Voss. An Arnoldi method for nonlinear eigenvalue problems. *BIT*, 44(2):387–401, 2004.

[39] H. Voss. Iterative projection methods for computing relevant energy states of a quantum dot. *J. Comput. Phys.*, 217(2):824–833, 2006.

[40] H. Voss. A Jacobi-Davidson method for nonlinear and nonsymmetric eigenproblems. *Comput. & Structures*, 85(17-18):1284–1292, 2007.

[41] J. Wu. *Theory and applications of partial functional-differential equations*, volume 119 of *Applied Mathematical Sciences*. Springer, New York, 1996.