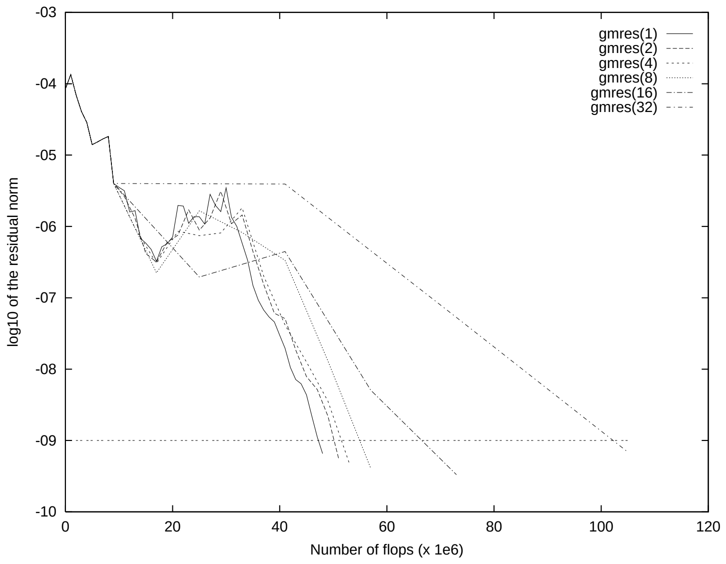

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Jacobi-Davidson Type Methods for Generalized Eigenproblems and Polynomial Eigenproblems: Part I

by

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JACOBI-DAVIDSON TYPE METHODS FOR GENERALIZED EIGENPROBLEMS AND POLYNOMIAL EIGENPROBLEMS: PART I

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Abstract. In this paper we will show how the Jacobi-Davidson iterative method can be used to solve generalized eigenproblems. Similar ideas as for the standard eigenproblem are used, but the projections, that are required to reduce the given problem to a small manageable size, need more attention. We show that by proper choices for the projection operators quadratic convergence can be achieved. The advantage of our approach is that none of the involved operators needs to be inverted. It turns out that similar projections can be used for the iterative approximation of selected eigenvalues and eigenvectors of polynomial eigenvalue equations. This approach has already been used with great success for the solution of quadratic eigenproblems associated with acoustic problems.

Key words. Eigenvalues and eigenvectors, eigenproblem, generalized eigenproblem, quadratic eigenproblem, polynomial eigenproblem, Jacobi-Davidson method, Ritz values, harmonic Ritz values.

AMS subject classification. 65F15, 65N25.

Our friend Albert died on November 12, 1995

1. Introduction.

The Jacobi-Davidson method [28] constructs iteratively approximations of certain eigenvectors. It finds the approximate eigenvector as "best" approximations in some search space.

In this paper we are interested in numerical methods to compute accurate approximations of the solutions $(\mu, \lambda, \mathbf{x})$ of the following generalized eigenvalue problem

$$\mu \mathbf{A}\mathbf{x} = \lambda\, \mathbf{B}\mathbf{x}, \tag{1}$$

where $\mathbf{A}$ and $\mathbf{B}$ are $n \times n$ matrices, $\mathbf{x}$ is a non-trivial n-vector and (μ, λ) is an element in the one dimensional complex projective plane (one may think of μ and λ in the complex plane, scaled such that $\mu \in [0,1]$ and $|\mu|^2 + |\lambda|^2 = 1$). Typically, n is large and $\mathbf{A}$ and $\mathbf{B}$ are sparse.

For the moment, for ease of presentation, we assume $\mathbf{B}$ to be non-singular and we scale μ to be 1 and take $\lambda \in \mathbb{C}$.

General remarks. Observe that both the eigenproblem $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, as well as the inverse eigenproblem $(1/\lambda)\mathbf{x} = \mathbf{A}^{-1}\mathbf{x}$ (assuming that $\mathbf{A}$ is non-singular) fit in the frame of the generalized eigenproblem.

Conversely, for non-singular $\mathbf{B}$, the generalized eigenproblem can be formulated as a eigenproblem, $\mathbf{B}^{-1}\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ or $\mathbf{A}\mathbf{B}^{-1}\mathbf{w} = \lambda\mathbf{w}$ with $\mathbf{x} = \mathbf{B}\mathbf{w}$.

If $\mathbf{B}$ is positive definite, then, in order to maintain a possible symmetry of the matrix $\mathbf{A}$, one might wish to represent the generalized eigenproblem as a eigenproblem of $\mathbf{B}^{-\frac{1}{2}}\mathbf{A}\mathbf{B}^{-\frac{1}{2}}$: $\mathbf{B}^{-\frac{1}{2}}\mathbf{A}\mathbf{B}^{-\frac{1}{2}}\mathbf{w} = \lambda\mathbf{w}$ with $\mathbf{x} = \mathbf{B}^{-\frac{1}{2}}\mathbf{w}$.

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Since the generalized eigenproblem is "symmetric" in $\mathbf{A}$ and $\mathbf{B}$, similar observations can be made, interchanging $\mathbf{A}$ and $\mathbf{B}$, in case $\mathbf{A}$ is non-singular or positive definite.

2. The updating process for the approximate eigenvector. Suppose we have a non-trivial approximation $\mathbf{u}$ of an eigenvector $\mathbf{x}$ with approximation ϑ of the eigenvalue λ associated to $\mathbf{x}$ for which

$$\mathbf{r} := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u} \perp \mathbf{u}.$$

We look for an update $\mathbf{z}$ for $\mathbf{u}$ in the space orthogonal to $\mathbf{u}$; that is we are interested in

$$\text{(2)} \qquad \mathbf{z} \perp \mathbf{u} \quad \text{for which} \quad \mathbf{A}(\mathbf{u}+\mathbf{z}) = \lambda\,\mathbf{B}(\mathbf{u}+\mathbf{z}),$$

and $\mathbf{x}$ is a scalar multiple of $\mathbf{u}+\mathbf{z}$. With

$$\alpha := \frac{(\mathbf{A}\mathbf{u},\mathbf{u})}{(\mathbf{u},\mathbf{u})}, \quad \mathbf{a} := \mathbf{A}\mathbf{u} - \alpha\mathbf{u}, \quad \beta = \frac{(\mathbf{B}\mathbf{u},\mathbf{u})}{(\mathbf{u},\mathbf{u})}, \quad \mathbf{b} := \mathbf{B}\mathbf{u} - \beta\mathbf{u},$$

problem (2) is equivalent to the following pair of coupled equations:

$$\text{(3)} \qquad \begin{cases} \text{(a)} & \lambda = \dfrac{\mathbf{u}^*\mathbf{A}(\mathbf{u}+\mathbf{z})}{\mathbf{u}^*\mathbf{B}(\mathbf{u}+\mathbf{z})}, \\[2ex] \text{(b)} & \mathbf{z} \perp \mathbf{u} \quad \text{and} \quad \left(\mathbf{I} - \dfrac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \lambda\,\mathbf{B})\big|_{\mathbf{u}^\perp}\mathbf{z} = -(\mathbf{a} - \lambda\mathbf{b}). \end{cases}$$

Note that α, β, $\mathbf{a}$ and $\mathbf{b}$ can be readily computed. Moreover,

$$\vartheta = \frac{\alpha}{\beta} \quad \text{and} \quad \mathbf{r} = \mathbf{a} - \vartheta\mathbf{b}.$$

Following a suggestion made by Jacobi [14] for the standard eigenproblem for diagonally dominant symmetric matrices, it was proposed for general matrices [28] to solve this system iteratively, computing λ_j ((3)(a)) with $\mathbf{z}$ replaced by $\mathbf{z}_j$, and computing $\mathbf{z}_{j+1}$ from (3)(b) with λ replaced by λ_j (*the Jacobi orthogonal correction method*).

With $\mathbf{z}_0 = \mathbf{0}$ as an initial guess we have that $\lambda_0 = \vartheta$ and that $\mathbf{z}_1$ is the solution of the following *correction equation.*

$$\text{(4)} \qquad \mathbf{z}_1 \perp \mathbf{u} \quad \text{and} \quad \left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)(\mathbf{A} - \vartheta\,\mathbf{B})\big|_{\mathbf{u}^\perp}\mathbf{z}_1 = -\mathbf{r}.$$

Since $\mathbf{z}_j$ is only an approximation for the exact correction $\mathbf{z}$ there is no need to solve (3)(b) (nor the one in (4)) very accurately: for instance, we may use a few steps of an iterative method to solve linear systems of equations (e.g., GMRES(m) [24] or Gauss–Jacobi [13], as Jacobi did for the symmetric standard eigenproblem [14]).

In the computation of this approximate $\mathbf{z}_j$, one may use the fact that

$$\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}\right)\mathbf{z} \perp \mathbf{u} \quad \text{for any} \quad \mathbf{z},$$

for the construction of an approximation $\mathbf{z}_j$ that is orthogonal to $\mathbf{u}$. The expression in (3)(a) offers the possibility to update the approximation of the eigenvalue during the phase of solving approximately the linear system in (3)(b).

In a related context, Davidson [6] pointed out (see also [28]) that the speed of convergence may be improved if we not restrict ourselves to simply finding the new approximation by correcting $\mathbf{u}^{(k)} = \mathbf{u}$ by an approximate correction $\mathbf{z}_j$, but instead try to identify the best approximation in the subspace spanned by the approximating eigenvectors $\mathbf{u}^{(0)}, \ldots, \mathbf{u}^{(k)}, \mathbf{u}^{(k)} + \mathbf{z}_j$ constructed so far. In [28] this approach was combined with the *Jacobi orthogonal correction method* for the iterative solution of standard unsymmetric eigenproblems. The advantages of this subspace approach are obvious. For computational reasons (efficiency, stability, ...), it is more convenient to use an orthogonal basis $\mathbf{v}_1, \ldots, \mathbf{v}_{k+1}$ of vectors that span the same subspace as the set of approximating eigenvectors. Note that $\{\mathbf{u}^{(k)}, \mathbf{u}^{(k)} + \mathbf{z}_\ell\}$ and $\{\mathbf{u}^{(k)}, \mathbf{z}_\ell\}$ span the same subspace. This leads to a strategy that will be further explained in Section 4.

If we update $\mathbf{u}$ in each step by the *exact* solution $\mathbf{z}_1$ of the correction equation (4) (that is, with $\mathbf{u}_k = \mathbf{u}$, in the next step we take $\mathbf{u} = \mathbf{u}_{k+1} = \mathbf{u}_k + \mathbf{z}_1$), then we have a process that converges asymptotically quadratical when $\mathbf{B} = \mathbf{I}$ (see TH. 3.2, or [28, Section 5]). To retain quadratic convergence also for the case where $\mathbf{B} \neq \mathbf{I}$, we have to adjust the projection $\mathbf{I} - \frac{\mathbf{u}\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}$. We will address the choice of the proper projection in the next section.

3. Other projections for the eigenvector approximations. Suppose we have an non-trivial approximation $\mathbf{u}$ of an eigenvector $\mathbf{x}$ with approximation ϑ of the eigenvalue λ associated to $\mathbf{x}$. Assume also that we have a vector $\mathbf{w}$ for which

$$\mathbf{r} := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u} \perp \mathbf{w}.$$

We look for an update $\mathbf{z}$ of $\mathbf{u}$ in the space orthogonal to some $\widetilde{\mathbf{u}}$ ($\widetilde{\mathbf{u}} \not\perp \mathbf{u}$): we are interested in

$$\text{(5)} \qquad \mathbf{z} \perp \widetilde{\mathbf{u}} \quad \text{for which} \quad \mathbf{A}(\mathbf{u} + \mathbf{z}) = \lambda\,\mathbf{B}(\mathbf{u} + \mathbf{z}).$$

As in Section 2 we have, except for a scalar multiple, $\mathbf{x} = \mathbf{u} + \mathbf{z}$. The introduction of $\widetilde{\mathbf{u}}$ is not so obvious at the moment, we could simply have taken the vector $\mathbf{u}$. It will appear that other choices for $\widetilde{\mathbf{u}}$ may be convenient, like $\widetilde{\mathbf{u}} = \mathbf{B}\mathbf{u}$.

For similar reasons we select a $\widetilde{\mathbf{w}} \not\perp \mathbf{w}$, and we consider the projections

$$\text{(6)} \qquad \mathbf{P} := \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}} \quad \text{and} \quad \mathbf{Q} := \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}.$$

The projection $\mathbf{Q}$ splits the space $\mathbb{C}^n$ into the subspace spanned by $\mathbf{u}$ and the orthogonal complement of $\widetilde{\mathbf{u}}$, that is, $\mathbf{v} = \mathbf{Q}\mathbf{v} + (\mathbf{I} - \mathbf{Q})\mathbf{v}$, $\mathbf{Q}\mathbf{v} = \gamma\mathbf{u}$ and $(\mathbf{I} - \mathbf{Q})\mathbf{v} \perp \widetilde{\mathbf{u}}$ for each $\mathbf{v}$. Similarly, the projection $\mathbf{P}$ splits the space into the subspace spanned by $\widetilde{\mathbf{w}}$ and the orthogonal complement of $\mathbf{w}$. The projections can also be used to decompose the eigenproblem:

$$\text{(7)} \qquad (\mathbf{A} - \lambda\,\mathbf{B})\mathbf{x} = 0 \;\Leftrightarrow\; \left\{ \begin{array}{r} \mathbf{P}(\mathbf{A} - \lambda\,\mathbf{B})(\mathbf{Q}\mathbf{x} + (\mathbf{I} - \mathbf{Q})\mathbf{x}) = 0 \quad \& \\ (\mathbf{I} - \mathbf{P})(\mathbf{A} - \lambda\,\mathbf{B})(\mathbf{Q}\mathbf{x} + (\mathbf{I} - \mathbf{Q})\mathbf{x}) = 0. \end{array} \right.$$

With

$$\text{(8)} \qquad \alpha := \frac{(\mathbf{A}\mathbf{u}, \mathbf{w})}{(\mathbf{u}, \mathbf{w})}, \quad \mathbf{a} := \mathbf{A}\mathbf{u} - \alpha\mathbf{u}, \quad \beta := \frac{(\mathbf{B}\mathbf{u}, \mathbf{w})}{(\mathbf{u}, \mathbf{w})}, \quad \mathbf{b} := \mathbf{B}\mathbf{u} - \beta\mathbf{u},$$

and

$$\mathbf{u}' := \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)\mathbf{u} = \mathbf{u} - \frac{(\mathbf{u},\mathbf{w})}{(\widetilde{\mathbf{w}},\mathbf{w})}\widetilde{\mathbf{w}}$$

we now see that problem (5) is equivalent to the following problem.

$$(9)\qquad \begin{cases} \text{(a)} & \lambda = \dfrac{\mathbf{w}^*\mathbf{A}\,(\mathbf{u}+\mathbf{z})}{\mathbf{w}^*\mathbf{B}\,(\mathbf{u}+\mathbf{z})}, \\ \text{(b)} & \mathbf{z} \perp \widetilde{\mathbf{u}} \quad \text{and} \\ & \left(\mathbf{I} - \dfrac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)(\mathbf{A} - \lambda\,\mathbf{B})\big|_{\widetilde{\mathbf{u}}^\perp}\mathbf{z} = -(\mathbf{a} - \lambda\mathbf{b}) - (\alpha - \lambda\beta)\mathbf{u}'. \end{cases}$$

The quantities α, β, $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{u}'$ can be easily computed. Moreover,

$$(10)\qquad \vartheta = \frac{\alpha}{\beta} \quad \text{and} \quad \mathbf{r} = \mathbf{a} - \vartheta\mathbf{b} = \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u}.$$

Note that $\mathbf{r} \perp \mathbf{w}$.

If we solve equation (9(b)) only approximately by replacing λ by the approximation ϑ, then we arrive at the following correction equation:

$$(11)\qquad \text{(a)}\quad \mathbf{z} = \left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z} \qquad \text{and} \qquad \text{(b)}\quad \mathbf{F}_p\,\mathbf{z} = -\mathbf{r},$$

where

$$(12)\qquad \mathbf{F}_p := \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)(\mathbf{A} - \vartheta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right).$$

This suggests the iterative process as described in ALGORITHM 1: compute an approximate solution $\mathbf{z}_1$ from equation (11(b)); update $\mathbf{u}$, (i.e., $\mathbf{u}_{\text{new}} = \mathbf{u}_{\text{old}} + \mathbf{z}_1$); choose appropriate of $\mathbf{w}$, $\widetilde{\mathbf{u}}$, and $\widetilde{\mathbf{w}}$, in order to satisfy the non-orthogonality conditions for these vectors, and repeat the procedure until the approximate eigenvector $\mathbf{u}$ is accurate enough. If the correction equation is solved exactly, then, according to the following theorems, THEOREM 3.2 and THEOREM 3.9, we may expect superlinear, and even quadratic convergence, depending on the choices of the $\mathbf{w}$, $\widetilde{\mathbf{u}}$ and $\widetilde{\mathbf{w}}$.

3.1. Fast convergence with right eigenvectors. In this section λ is assumed to be a simple eigenvalue of $\mathbf{A}\mathbf{B}^{-1}$ with eigenvector $\mathbf{x} \neq 0$ of the generalized eigenproblem: $(\mathbf{A} - \lambda\,\mathbf{B})\mathbf{x} = 0$.

LEMMA 3.1. *Consider* $\mathbf{w}$ *and* $\widetilde{\mathbf{u}}$ *for which* $\widetilde{\mathbf{u}}^*\mathbf{x} \neq 0$ *and* $(\mathbf{B}\mathbf{x})^*\mathbf{w} \neq 0$. *Then, the map*

$$\mathbf{F}_p := \left(\mathbf{I} - \frac{\mathbf{B}\mathbf{x}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{x}}\right)(\mathbf{A} - \lambda\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{x}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{x}}\right)$$

is a bijection from $\widetilde{\mathbf{u}}^\perp$ *onto* $\mathbf{w}^\perp$.

Proof. Suppose $\mathbf{y} \perp \widetilde{\mathbf{u}}$ and $\mathbf{F}_p\mathbf{y} = 0$. Then $(\mathbf{A} - \lambda\,\mathbf{B})\mathbf{y}$ is a scalar multiple of $\mathbf{B}\mathbf{x}$, and both $\mathbf{B}\mathbf{y}$ and $\mathbf{B}\mathbf{x}$ belong to the kernel of $(\mathbf{A}\mathbf{B}^{-1} - \lambda\,\mathbf{I})^2$.

The simplicity of λ implies that $\mathbf{B}\mathbf{y}$ is a scalar multiple of $\mathbf{B}\mathbf{x}$, and hence $\mathbf{y}$ is a multiple of $\mathbf{x}$. The fact that $\mathbf{y} \perp \widetilde{\mathbf{u}}$ and $\widetilde{\mathbf{u}}^*\mathbf{x} \neq 0$ implies $\mathbf{y} = 0$, which proves the injectivity of $\mathbf{F}_p$. An obvious dimension argument implies bijectivity. ☐

ALGORITHM 1. *The basic algorithm*

Choose a non-trivial $\mathbf{u}$

Repeat:

(a) Select a $\mathbf{w}$.

(b) Compute $\vartheta := \dfrac{\mathbf{w}^*\mathbf{A}\mathbf{u}}{\mathbf{w}^*\mathbf{B}\mathbf{u}}$ and $\mathbf{r} := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u}$.

(c) *Stop.* Stop if $\mathbf{u}$ and ϑ are accurate enough.

(d) Select a $\widetilde{\mathbf{u}}$ and a $\widetilde{\mathbf{w}}$.

(e) *Solve the correction equation (approximately).* Compute an approximate solution $\mathbf{z}_1 \perp \widetilde{\mathbf{u}}$ of the correction equation

$$\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)(\mathbf{A} - \vartheta\,\mathbf{B})\big|_{\widetilde{\mathbf{u}}^\perp}\mathbf{z} = -\mathbf{r}.$$

(f) *Update* $\mathbf{u}$. $\mathbf{u}' := \mathbf{u} + \mathbf{z}_1, \quad \mathbf{u} := \mathbf{u}'/\|\mathbf{u}'\|$.

The vectors $\widetilde{\mathbf{u}}$ and $\mathbf{w}$ can be chosen differently in each step, and one has to do this carefully in order to ensure the non-orthogonality conditions. One can work with the same vectors at the risk of a breakdown and we will discuss more robust choices in our discussion after the next theorem. We need that these vectors converge in order to be able to make statements on the convergence of the approximations $\mathbf{u}$.

THEOREM 3.2. *Assume that the correction equation is solved exactly in each step of* ALGORITHM 1. *Choose* $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$ *in each step. Assume that the* $\widetilde{\mathbf{u}}$ *and* $\mathbf{w}$ *converge and that both* $\widetilde{\mathbf{u}}^*\mathbf{x}$ *and* $\mathbf{w}^*\mathbf{B}\mathbf{x}$ *have non-trivial limits.*

Then, if the initial vector $\mathbf{u}$ *is close enough to* $\mathbf{x}$*, the sequence of* $\mathbf{u}$ *convergences in direction to* $\mathbf{x}$ *and the sequence of* $\vartheta = \mathbf{w}^*\mathbf{A}\mathbf{u}/\mathbf{w}^*\mathbf{B}\mathbf{u}$ *converges to* λ.

If the $\mathbf{u}$ *converge in direction to* $\mathbf{x}$ *then the convergence is quadratical.*

Proof. Suppose $(\mathbf{A} - \lambda\,\mathbf{B})\mathbf{x} = 0$ with $\mathbf{x}$ such that $\mathbf{x} = \mathbf{u} + \mathbf{z}$ for $\mathbf{z} \perp \widetilde{\mathbf{u}}$. Then

$$(\mathbf{A} - \vartheta\,\mathbf{B})\mathbf{z} = -(\mathbf{A} - \vartheta\,\mathbf{B})\mathbf{u} + (\lambda - \vartheta)\mathbf{B}\mathbf{x} = -\mathbf{r} + (\lambda - \vartheta)\mathbf{B}\mathbf{x}. \tag{13}$$

Consider the exact solution $\mathbf{z}_1 \perp \widetilde{\mathbf{u}}$ of the correction equation:

$$(\mathbf{I} - \mathbf{P})(\mathbf{A} - \vartheta\,\mathbf{B})\mathbf{z}_1 = -(\mathbf{I} - \mathbf{P})\mathbf{r} = -\mathbf{r} \tag{14}$$

(remember that $\mathbf{r} \perp \mathbf{w}$). Since $\mathbf{x} - (\mathbf{u} + \mathbf{z}_1) = \mathbf{z} - \mathbf{z}_1$ and $\mathbf{z} = \mathbf{u} - \mathbf{x}$, for quadratic convergence, it suffices to show that

$$\|\,\mathbf{z} - \mathbf{z}_1\| = \mathcal{O}(\|\,\mathbf{z}\,\|^2).$$

Multiplying (13) by $(\mathbf{I} - \mathbf{P})$ and subtracting the result from (14) yields

$$(\mathbf{I} - \mathbf{P})(\mathbf{A} - \vartheta\,\mathbf{B})(\mathbf{z} - \mathbf{z}_1) = (\lambda - \vartheta)(\mathbf{I} - \mathbf{P})\mathbf{B}\mathbf{z} + (\lambda - \vartheta)(\mathbf{I} - \mathbf{P})\mathbf{B}\mathbf{u}. \tag{15}$$

Multiplying (13) by $\mathbf{w}^*$ and using that $\mathbf{r} \perp \mathbf{w}$ leads to

$$\lambda - \vartheta = \frac{\mathbf{w}^*(\mathbf{A} - \vartheta\,\mathbf{B})\mathbf{z}}{\mathbf{w}^*\mathbf{B}\mathbf{x}}. \tag{16}$$

Since, by assumption, $\mathbf{w}^*\mathbf{B}\mathbf{x}$ has a non-trivial limit, we obtain

$$\|(\lambda - \vartheta)(\mathbf{I} - \mathbf{P})\mathbf{B}\,\mathbf{z}\| = \mathcal{O}(\|\,\mathbf{z}\,\|^2).$$

Because of (15), this implies quadratic convergence, if $(\mathbf{I} - \mathbf{P})(\mathbf{A} - \vartheta\,\mathbf{B})_{|\widetilde{\mathbf{u}}^\perp}$ is non-singular and $(\mathbf{I} - \mathbf{P})\mathbf{B}\mathbf{u} = 0$. This last condition holds since $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$. The non-singularity follows from LEMMA 3.1 and the assumption that the sequences of $\mathbf{u}$, $\mathbf{w}$ and $\widetilde{\mathbf{u}}$ have limits. □

We will now make some remarks with respect to the choices for $\widetilde{\mathbf{w}}$, $\mathbf{w}$, and $\widetilde{\mathbf{u}}$.

REMARK 3.3. If the sequence of approximate eigenvectors $\mathbf{u}$ converges then $\mathbf{A}\mathbf{u} \approx \lambda\,\mathbf{B}\mathbf{u}$, and the choice $\widetilde{\mathbf{w}} = \vartheta\,\mathbf{A}\mathbf{u} + \mathbf{B}\mathbf{u}$ also leads to a quadratic convergent process.

REMARK 3.4. If $\widetilde{\mathbf{u}}$ and $\mathbf{w}$ are kept fixed during the iterative process, the sequences of vectors $\widetilde{\mathbf{u}}$ and $\mathbf{w}$ clearly converge. In this case, we are looking for an eigenvector $\mathbf{x}$ with non-trivial component in the direction $\widetilde{\mathbf{u}}$ (the condition $\widetilde{\mathbf{u}}^*\mathbf{x} \neq 0$) and we hope to find this vector by keeping the residual orthogonal to $\mathbf{w}$. As mentioned earlier, there is no guarantee that all the inner products involved in the projections $\mathbf{P}$ and $\mathbf{Q}$ do not vanish.

Inspection of the arguments in the proof of THEOREM 3.2 reveals that a choice of $\widetilde{\mathbf{u}}$ and $\mathbf{w}$ correlated to $\mathbf{u}$, as $\widetilde{\mathbf{u}} = \mathbf{w} = \mathbf{u}$ or as $\widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{u}$, $\mathbf{w} = \mathbf{u}$, leads to converging sequences provided that the initial guess $\mathbf{u}$ is sufficiently close to $\mathbf{x}$ and provided that the limit inner products are non-zero ($\mathbf{x}^*\mathbf{B}\mathbf{x} \neq 0$).

EXAMPLES 3.5. (a) For some $\nu \in \{1, \ldots, n\}$, for the case where $\mathbf{B} = \mathbf{I}$, Jacobi's method [14] comes down to the choice $\widetilde{\mathbf{u}} = \mathbf{w} = \widetilde{\mathbf{w}} = e_\nu$, leading to a linearly convergent process.

The Jacobi-Davidson processes can be interpreted as Newton processes for suitable choices of the vectors involved [29]. We give two examples.

(b1) The choice $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$ and both $\widetilde{\mathbf{u}}$ and $\mathbf{w}$ fixed throughout the iteration process leads to a method that is equivalent to the Newton's process (see Sect. 7.2) applied to equation

$$r(\mathbf{u}) := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u} = 0 \quad \text{with} \quad (\mathbf{u}, \widetilde{\mathbf{u}}) = 1 \quad \text{and} \quad \vartheta \text{ such that } r(\mathbf{u}) \perp \mathbf{w}. \tag{17}$$

(b2) The choice $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, $\widetilde{\mathbf{u}} = \mathbf{u}$, and $\mathbf{w} = \mathbf{u}$ leads to a method that is equivalent to Newton's method applied to equation

$$r(\vartheta, \mathbf{u}) := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u} = 0 \quad \text{with} \quad \|\mathbf{u}\| = 1. \tag{18}$$

For more details, see Appendix A.

(c) The choice $\widetilde{\mathbf{u}} = \mathbf{w} = \widetilde{\mathbf{w}} = \mathbf{u}$ is elegant because of its simplicity, but it only leads to an asymptotically quadratically convergent process if $\mathbf{B} = \mathbf{I}$. The fact that this choice does not lead to quadratic convergence in general if $\mathbf{B} \neq \tau\mathbf{I}$, expresses the more complicated nature of general eigenproblems. This follows from the requirement that $(\mathbf{I} - \mathbf{P})\mathbf{B}\mathbf{u} = 0$, which implies that $\mathbf{B}\mathbf{u}$ should a multiple of $\widetilde{\mathbf{w}}$.

REMARK 3.6. The choice $\widetilde{\mathbf{w}} = \mathbf{u}$ leads to asymptotic quadratic convergence when applied to the eigenproblem $\mathbf{B}^{-1}\mathbf{A}$. However, by choosing $\mathbf{w} = \mathbf{B}^*\mathbf{w}'$ and multiplying the correction equation for the eigenproblem $\mathbf{B}^{-1}\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ to the left by $\mathbf{B}$, we arrive precisely at the correction equations as discussed above.

3.2. Fast convergence with left eigenvectors. In the previous section we discussed fast convergence for the case where $\widetilde{\mathbf{w}}$ converges to a (right) eigenvector of $\mathbf{A}\mathbf{B}^{-1}$. As we will see in this section, we may also expect fast convergence if the $\mathbf{w}$ converge to a left eigenvector of $\mathbf{A} - \lambda\,\mathbf{B}$. This approach allows the choice of more natural projections: $\mathbf{P}$ may be selected to be equal to $\mathbf{Q}$ (this will be further exploited in Section 3.3).

Similar arguments as in the proof of LEMMA 3.1 lead to the following lemma.

LEMMA 3.7. *The map*

$$\mathbf{F}_p := \left(\mathbf{I} - \frac{\mathbf{x}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{x}}\right)(\mathbf{A} - \lambda\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{x}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{x}}\right), \tag{19}$$

is also a bijection from $\widetilde{\mathbf{u}}^\perp$ *onto* $\mathbf{w}^\perp$ *if* 0 *is a simple eigenvalue of* $\mathbf{A} - \lambda\,\mathbf{B}$.

REMARK 3.8. The scalar ϑ is a simple eigenvalue of the general eigenproblem if ϑ is a single root of the characteristic polynomial $\det(\mathbf{A} - \lambda\,\mathbf{B})$, or, equivalently, if ϑ is a simple eigenvalue of the matrix $\mathbf{A}\mathbf{B}^{-1}$ (recall that $\mathbf{B}$ is non-singular by assumption). However, in general this does not imply that 0 is a simple eigenvalue of the eigenproblem for the matrix $\mathbf{A} - \vartheta\,\mathbf{B}$. Although the geometrical multiplicity is one, the algebraic multiplicity can be larger. If the geometric and the algebraic multiplicity coincide, for instance if both $\mathbf{A}$ and $\mathbf{B}$ are self-adjoint ($\mathbf{A}^* = \mathbf{A}$ and $\mathbf{B}^* = \mathbf{B}$), and ϑ is real, then 0 is a simple eigenvalue of $\mathbf{A} - \vartheta\,\mathbf{B}$ when ϑ is a simple eigenvalue of $\mathbf{A}\mathbf{B}^{-1}$.

THEOREM 3.9. *Assume that* 0 *is a simple eigenvalue of* $\mathbf{A} - \lambda\,\mathbf{B}$.
Assume that, in each step of ALGORITHM 1*, the correction equation is solved exactly. Assume the* $\widetilde{\mathbf{u}}$*'s,* $\mathbf{w}$*'s and* $\widetilde{\mathbf{w}}$*'s converge,* $\widetilde{\mathbf{u}}^*\mathbf{u}$*,* $\widetilde{\mathbf{w}}^*\mathbf{w}$ *and* $\mathbf{w}^*\mathbf{B}\mathbf{u}$ *have non-trivial limits and* $(\mathbf{A} - \vartheta\,\mathbf{B})^*\mathbf{w}$ *converges towards* 0.

The $\mathbf{u}$ *convergence in direction to* $\mathbf{x}$ *if the initial vector* $\mathbf{u}$ *is close enough to* $\mathbf{x}$.

If the $\mathbf{u}$ *converge in direction to* $\mathbf{x}$ *then the convergence is superlinear.*

Proof. The assumptions and (16) imply that $|\lambda - \vartheta| = o(\|\,\mathbf{z}\,\|)$ and, as in the proof of Theorem 3.2, superlinear convergence follows from (15). □

REMARK 3.10. If both $\mathbf{A}$ and $\mathbf{B}$ are self adjoint and $\lambda \in \mathbb{R}$ then, for the choice $\mathbf{w} = \mathbf{u}$, we have that $\mathbf{w}^*(\mathbf{A} - \lambda\,\mathbf{B}) = -\mathbf{z}^*(\mathbf{A} - \lambda\,\mathbf{B})$. Therefore, in this "symmetric case", we have that

$$|\lambda - \vartheta| = \mathcal{O}(\|\,\mathbf{z}\,\|^2), \tag{20}$$

which implies quadratic convergence for any choice of $\widetilde{\mathbf{w}}$.

REMARK 3.11. More general, we obtain quadratic convergence if we select our $\mathbf{w}$ to converge to the left eigenvector of $\mathbf{A} - \lambda\,\mathbf{B}$, by an obvious adjoint version of ALGORITHM 1, that is:
with $\mathbf{r}_\ell := (\mathbf{A} - \vartheta\,\mathbf{B})^*\mathbf{w}$, solve exactly the adjoint correction equation:

$$\mathbf{z}_\ell \perp \widetilde{\mathbf{w}} \quad \text{such that} \quad \mathbf{z}_\ell^*\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)(\mathbf{A} - \vartheta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right) = -\mathbf{r}_\ell^*, \tag{21}$$

and update $\mathbf{w}$ similar to $\mathbf{u}$: $\mathbf{w}' := \mathbf{w} + \mathbf{z}_\ell$, $\mathbf{w} := \mathbf{w}'/\|\mathbf{w}'\|$. Note that $\mathbf{r}_\ell \perp \mathbf{u}$.

With this approach we also have converging $\mathbf{u}$, $\mathbf{w}$, $\widetilde{\mathbf{u}}$, and $\widetilde{\mathbf{w}}$, if the initial $\mathbf{u}$ is close enough to $\mathbf{x}$, the initial $\mathbf{w}$ is close enough to the left eigenvector of $\mathbf{A} - \lambda\,\mathbf{B}$, and $\widetilde{\mathbf{u}}$, $\widetilde{\mathbf{w}}$ are fixed or $\widetilde{\mathbf{u}} = \mathbf{w}$, $\widetilde{\mathbf{w}} = \mathbf{u}$, and the non-zero conditions on the inner products are fulfilled.

We obtain cubic convergence if, in addition, we choose $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$.

3.3. The choice of the projections P and Q. If $\mathbf{w} \neq \widetilde{\mathbf{u}}$ then the domain space $\widetilde{\mathbf{u}}^{\perp}$ of the map $\mathbf{F}_p$ in (12) differs from the image space $\mathbf{w}^{\perp}$ of this map $\mathbf{F}_p$. Powers of $\mathbf{F}_p$ cannot be formed, and to solve equation (11) by some Krylov subspace method, we need a "preconditioner" $\mathbf{K}$ that maps the image space $\mathbf{w}^{\perp}$ bijectively onto the domain space $\widetilde{\mathbf{u}}^{\perp}$: then we can apply Krylov subspace methods to the preconditioned system (see Sect. 7.1). In other words, for unpreconditioned Krylov subspace methods, it is desirable to have $(\mathbf{I}-\mathbf{P})(\mathbf{I}-\mathbf{Q}) = \mathbf{I}-\mathbf{Q}$, or, equivalently, $\widetilde{\mathbf{u}} = \mathbf{w}$.

The choice $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, $\widetilde{\mathbf{u}} = \mathbf{w}$ leads to a fast converging process in which the correction equation requires a solution in the space that also contains the residual.

The choice $\widetilde{\mathbf{w}} = \mathbf{u}$, $\widetilde{\mathbf{u}} = \mathbf{w}$ and $\mathbf{w}$ some approximate left eigenvector leads to fast convergence (cf. Sect. 3.2), and the projections $\mathbf{P}$ and $\mathbf{Q}$ coincide. If 0 is a simple eigenvalue of $\mathbf{A} - \lambda\,\mathbf{B}$, and $\mathbf{u}$ and $\mathbf{w}$ converge to the associated right and left eigenvector, respectively, then $\widetilde{\mathbf{w}}^*\mathbf{w} = \mathbf{u}^*\mathbf{w}$ has a non-trivial limit value.

By embedding the correction equation into the entire space $\mathbb{C}^n$, we also circumvent the problem of having an domain space that differs from the image space: in the whole space, we trivially have the same image and domain space. For instance, the choice $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, $\widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{w}$, implies $\mathbf{B}\mathbf{Q} = \mathbf{P}\mathbf{B}$. Hence, $(\mathbf{I}-\mathbf{P})\mathbf{B} = (\mathbf{I}-\mathbf{P})\mathbf{B}(\mathbf{I}-\mathbf{Q})$. Since $\mathbf{r} = (\mathbf{I}-\mathbf{P})\mathbf{r}$, the solution $\mathbf{z}$ of problem (11) is precisely $\mathbf{z} = (\mathbf{I}-\mathbf{Q})\widetilde{\mathbf{z}}$ where $\widetilde{\mathbf{z}} \in \mathbb{C}^n$ is the solution of the equation

$$(22) \qquad (\mathbf{A}_p - \vartheta\,\mathbf{B})\,\widetilde{\mathbf{z}} = -\mathbf{r} \quad \text{where} \quad \mathbf{A}_p := \left(\mathbf{I} - \frac{\mathbf{B}\mathbf{u}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{u}}\right)\mathbf{A}\left(\mathbf{I} - \frac{\mathbf{u}\,\mathbf{w}^*\mathbf{B}}{\mathbf{w}^*\mathbf{B}\mathbf{u}}\right).$$

The embedded equation in (22) is non-singular if the equation in (11) is non-singular, $\vartheta \neq 0$ and $\beta \neq 0$ (or, equivalently, $\mathbf{w}^*\mathbf{B}\mathbf{u} \neq 0$).

The choice $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, $\widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{w}$, leads to a fast converging process and the correction equation can be embedded in the entire space. If, in addition, $\mathbf{w} = \mathbf{u}$ and $\mathbf{B}$ is self-adjoint then $\mathbf{P}^* = \mathbf{Q}$. With $\mathbf{w} = \widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$ and $\widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{B}\mathbf{u}$ the inner product $\widetilde{\mathbf{w}}^*\mathbf{w} = \widetilde{\mathbf{u}}^*\mathbf{u}$ $(= \|\mathbf{B}\mathbf{u}\|^2)$ is non-zero. This is also the case if $\mathbf{B}$ is positive definite and $\mathbf{w} = \mathbf{u}$.

3.4. Equivalent formulations for the correction equation. The dimension of the problem defined by the correction equation (11) is smaller than the dimension of the space of the eigenproblem: the projections are used to restrict the image space and domain space to a space of co-dimension 1. As is stated by the following theorem, the projections can also be used for an equivalent formulation in a space of larger dimension. This equivalent augmented formulation may be useful for the construction of preconditioners for the correction equation (11) (cf. Sect. 7.1). For similar reasons [9], such an augmented equation also appears in the theory for numerical continuation methods for nonlinear equations (cf., e.g., [10]).

THEOREM 3.12. *Equation* (11) *is equivalent to*

$$\begin{bmatrix} \mathbf{A}-\vartheta\,\mathbf{B} & \widetilde{\mathbf{w}} \\ \widetilde{\mathbf{u}}^* & 0 \end{bmatrix} \begin{bmatrix} \mathbf{z} \\ \varepsilon \end{bmatrix} = \begin{bmatrix} -\mathbf{r} \\ 0 \end{bmatrix}, \tag{23}$$

that is, $\mathbf{z}$ *is a solution of* (23) *if and only if* $\mathbf{z}$ *is a solution of* (11).

Proof. Obviously, equation (23) implies that $\widetilde{\mathbf{u}}^*\mathbf{z} = 0$, and this holds if and only if $\mathbf{z} \perp \widetilde{\mathbf{u}}$.

Since $\mathbf{r} \perp \mathbf{w}$, the first block coordinate $(\mathbf{A}-\vartheta\,\mathbf{B})\mathbf{z}+\varepsilon\widetilde{\mathbf{w}} = -\mathbf{r}$ in (23) is equivalent to

$$\begin{cases} \left(\mathbf{I} - \dfrac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)((\mathbf{A}-\vartheta\,\mathbf{B})\,\mathbf{z}+\varepsilon\widetilde{\mathbf{w}}) = -\mathbf{r} \quad \text{and} \\ \mathbf{w}^*((\mathbf{A}-\vartheta\,\mathbf{B})\,\mathbf{z}+\varepsilon\widetilde{\mathbf{w}}) = 0. \end{cases} \tag{24}$$

Since $\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)\widetilde{\mathbf{w}} = 0$, we see that the first equation in (24) is equivalent to (11). The second equation determines ε $(= \mathbf{w}^*(\mathbf{A}-\vartheta\,\mathbf{B})\mathbf{z}/\mathbf{w}^*\widetilde{\mathbf{w}})$. $\square$

REMARK 3.13. In (11), the vectors $\mathbf{u}$ and $\mathbf{w}$ play a role. These vectors do not occur in equation (23). However, they enter through $\mathbf{r} = (\mathbf{A}-\vartheta\,\mathbf{B})\mathbf{u}$ and the condition $\mathbf{r} \perp \mathbf{w}$.
For the construction of incomplete factorizations that may serve as preconditioners it may be advantageous to reorder the equations in (23).

Using the fact that $\mathbf{r} = (\mathbf{A}-\vartheta\,\mathbf{B})\mathbf{u}$, (23), and therefore (11), can be solved exactly in terms of the solution $\mathbf{t}$ of the equation $(\mathbf{A}-\vartheta\,\mathbf{B})\mathbf{t} = \widetilde{\mathbf{w}}$:

THEOREM 3.14. *The solution* $\mathbf{z}$ *of* (11) *(and of* (23)*) is given by*

$$\mathbf{z} = -\mathbf{u} + \varepsilon\,(\mathbf{A}-\vartheta\,\mathbf{B})^{-1}\widetilde{\mathbf{w}} \quad \textit{with} \quad \varepsilon = \frac{\widetilde{\mathbf{u}}^*\mathbf{u}}{\widetilde{\mathbf{u}}^*(\mathbf{A}-\vartheta\,\mathbf{B})^{-1}\widetilde{\mathbf{w}}}. \tag{25}$$

Proof. With $\mathbf{z}$ as in (25), it is easily verified that $\widetilde{\mathbf{u}} \perp \mathbf{z}$ and $(\mathbf{A}-\vartheta\,\mathbf{B})\mathbf{z} = -\mathbf{r}+\varepsilon\widetilde{\mathbf{w}}$. Since $\mathbf{r} \perp \mathbf{w}$ it follows that (11) holds. $\square$

For $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, this theorem gives a relation to Rayleigh Quotient Iteration. In particular, we see that ALGORITHM 1 leads to cubical convergent sequences if $\mathbf{B} = \mathbf{I}$, $\mathbf{A}$ is symmetric, $\widetilde{\mathbf{u}} = \mathbf{w} = \widetilde{\mathbf{w}} = \mathbf{u}$, and if the correction equation is solved exactly, which is in agreement with observations made in Section 3.2. In Section 4 we use the approximate solution $\mathbf{z}$ to expand a subspace in which we search for new approximations for the eigenvector $\mathbf{x}$. This subspace will contain the current approximation $\mathbf{u}$ and expanding it by $\mathbf{z}$ (as in (25)) is equivalent to expanding it by $(\mathbf{A}-\vartheta\,\mathbf{B})^{-1}\widetilde{\mathbf{w}}$. For $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, this reveals a relation between the method to be discussed in Section 4 and Shift-and-Inverse Arnoldi; see DISCUSSION 4.1.

4. Projections on subspaces for approximating the eigenproblem. In the previous sections we have used projections $\mathbf{P}$ and $\mathbf{Q}$ defined with only single vectors $\widetilde{\mathbf{w}}$ and $\widetilde{\mathbf{u}}$. The older approximations were discarded, but following Davidson's approach, we will now take also these approximations into account, in order to prevent a search in a subspace that has already been explored. In this approach we store vectors that have been computed in previous steps, and we update $\mathbf{u}$ in the best way that is possible using all these vectors. The general *Jacobi-Davidson* (**JD**) algorithm, ALGORITHM 2, that we introduce in this section, is the basic ALGORITHM 1 with an improved updating strategy for the approximate eigenvector $\mathbf{u}$.

At the beginning of the kth step we have two sets of linearly independent vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ and $\mathbf{w}_1, \ldots, \mathbf{w}_k$. $\mathbf{V}_k$ is the matrix with the $\mathbf{v}_i$ as columns ($i = 1, \ldots, k$), $\mathcal{V}_k = \text{span}(\mathbf{V}_k)$, i.e., $\mathcal{V}_k$ is the subspace spanned by the columns $\mathbf{v}_i$ of $\mathbf{V}_k$. We use a similar notation $\mathbf{W}_k$ and $\mathcal{W}_k$ in relation to the $\mathbf{w}_i$. Then we construct our new approximating eigenvector $\mathbf{u}$, our new approximating eigenvalue ϑ by solving the *projected eigenproblem*:

$$\mathbf{u} \in \mathcal{V}_k, \quad \vartheta \in \mathbb{C} \qquad \text{that} \qquad \mathbf{r} := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u} \perp \mathcal{W}_k. \tag{26}$$

Since we look for the new approximate eigenvector in the subspace $\mathcal{V}_k$, we call $\mathcal{V}_k$ the *search space*. The subspace $\mathcal{W}_k$ is used in the projection to define an approximating problem. Analogously to the situation with Petrov-Galerkin methods, we will refer to $\mathcal{W}_k$ as the *test space*. Since this projected problem is equivalent to finding a $y \in \mathbb{C}^k$, $\vartheta \in \mathbb{C}$ such that

$$\mathbf{W}_k^*\mathbf{A}\mathbf{V}_k y - \vartheta\,\mathbf{W}_k^*\mathbf{B}\mathbf{V}_k y = 0 \quad \text{and} \quad \mathbf{u} = \mathbf{V}_k y \tag{27}$$

we only have to solve a small generalized eigenproblem of size k ($\mathbf{W}_k^*\mathbf{A}\mathbf{V}_k$ and $\mathbf{W}_k^*\mathbf{B}\mathbf{V}_k$ are $k \times k$ matrices) and compute $\mathbf{u}$ as a linear combination of the $\mathbf{v}_i$. We use the words *Petrov-Ritz value* for the approximate eigenvalue ϑ and *Petrov-Ritz vector* for the approximate eigenvector $\mathbf{u}$ (see also Sect. 5.1).

The approximate solution $\mathbf{z}_1$ of the correction equation (11) is used to expand the k-dimensional search space $\mathcal{V}_k$ to the space $\mathcal{V}_{k+1}$ of dimension $k+1$. Next, we select (or construct) a new $\mathbf{v}_{k+1}$ vector in the set of $\mathbf{v}_i$; $\mathbf{v}_{k+1}$ belongs to $\mathcal{V}_{k+1}$, and is linearly independent of $\mathbf{v}_1, \ldots, \mathbf{v}_k$. Finally, we construct a new $\mathbf{w}_{k+1}$. ALGORITHM 2 shows an algorithmical formulation of this strategy. In this formulation, we have suppressed the index k and we have included the possibility of reducing the search space and the test space (step (f)).

By expanding our subspace, we may expect better global convergence properties. But, moreover, we also may expect better local convergence. The choice $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$ (cf. TH. 3.2) leads to 'superquadratic' convergence (in analogy with the 'superlinear' convergence for Krylov subspace methods): the test space increases and will contain better approximations for the left eigenvector, which also leads to better approximations for ϑ (cf. (16), since in this case, by (26), for $\mathbf{w}$ we may take any vector in $\mathcal{W}_k$).

Any of the substeps (a)–(h) in this algorithm can be performed in a number of ways. Different choices in any of the substeps (b), (d), (f) and (h) lead to different sequences of approximating eigenvectors and eigenvalues. The specific choice of the basis vectors $\mathbf{v}_{k+1}$ and $\mathbf{w}_{k+1}$ in (g) and (h) affect the computational complexity and the stability of the algorithm. The choice of the spaces $\mathcal{V}_k$ (through (d), (e) and the restart strategy in (f)) and $\mathcal{W}_k$ (in (h)) affects the convergence behavior, while the choices of the basis of these space (in (g) and (h)) affect the computational complexity and the stability. We will comment on any of the substeps: on (a) in Section 6; (b) and (c) in Part II of this paper; (d) in Section 3; (e) in Section 7 (and 3); (f) in Part II; (g) and (h) in Section 5.

DISCUSSION 4.1. In order to keep our arguments simple, we will assume in this discussion that $\mathbf{B} = \mathbf{I}$. Furthermore, we will not consider restarts, and in ALGORITHM 2, we will take $\mathbf{W} = \mathbf{V}$, $\widetilde{\mathbf{w}} = \mathbf{u}$. $\mathbf{v}_1$ is the initial vector $\mathbf{v}$.

ALGORITHM 2. *The Jacobi-Davidson algorithm*

Choose a non-trivial $\mathbf{v}$ and a non-trivial $\mathbf{w}$.
Set $\mathbf{V} = [\mathbf{v}]$, $\mathbf{W} = [\mathbf{w}]$, $k = 0$.

Repeat:

(a) *Solve the projected eigenproblem.*
Compute non-trivial solutions $y \in \mathbb{C}^{k+1}$ and associated $\vartheta \in \mathbb{C}$ of the projected eigenproblem

$$\mathbf{W}^*\mathbf{A}\mathbf{V}\, y - \vartheta\, \mathbf{W}^*\mathbf{B}\mathbf{V}\, y = 0.$$

(b) *Select approximating eigenvector and eigenvalue.*
Select a solution y and associated Petrov-Ritz value ϑ.
Compute the Petrov-Ritz vector $\mathbf{u} \leftarrow \mathbf{V}y$ and the residual $\mathbf{r} \leftarrow \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u}$.

(c) *Stop.* Stop if $\mathbf{u}$ and ϑ are accurate enough.

(d) Select a $\mathbf{w}$ in span$(\mathbf{W})$ and select $\widetilde{\mathbf{u}}$ and $\widetilde{\mathbf{w}}$.

(e) *Solve the correction equation (approximately).*
Compute an approximate solution $\mathbf{z}_1 \perp \widetilde{\mathbf{u}}$ of the correction equation

$$\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)(\mathbf{A} - \vartheta\,\mathbf{B})\big|_{\widetilde{\mathbf{u}}^\perp}\mathbf{z} = -\mathbf{r}.$$

(f) *Restart.* $k \leftarrow$ dim(span$(\mathbf{V})$).
If k is too large:
select an $\ell < k$, select $k \times \ell$ matrices R_V and R_W,
compute $\mathbf{V} \leftarrow \mathbf{V}R_V$, $\mathbf{W} \leftarrow \mathbf{W}R_W$, $k \leftarrow \ell$.

(g) *Expand the search space.*
Select a $\mathbf{v} \in$ span$(\mathbf{V}, \mathbf{z}_1)\backslash$span$(\mathbf{V})$ and $\mathbf{V} \leftarrow [\mathbf{V}, \mathbf{v}]$.

(h) *Expand the test space.*
Select a $\widetilde{\mathbf{v}}$, $\widetilde{\mathbf{v}} \notin$ span$(\mathbf{W})$ and $\mathbf{W} \leftarrow [\mathbf{W}, \widetilde{\mathbf{v}}]$.

(a) ALGORITHM 2 can be interpreted as an improvement over Davidson's algorithm: in [6], Davidson formulated this algorithm (ALG. 2 with $\mathbf{W} = \mathbf{V}$) with a standard basis vector e_ν as initial vector $\mathbf{v}_1 = e_\nu$. As an approximate solution $\mathbf{z}_1$ of the correction equation he took $\mathbf{z}_1 = -(\mathrm{diag}(\mathbf{A} - \vartheta\,\mathbf{I}))^{-1}\mathbf{r}$, which is different from our projection approach. However, in connection with diagonal preconditioning, the projections may be discarded (cf. REMARK 7.2). Jacobi [14] took properly care of the projections (cf. EX. 3.5(a)), but did not accelerate by constructing a sequence of search spaces of increasing dimension. ALGORITHM 2 improves Davidson's approach as well as Jacobi's approach. Therefore, this new algorithm was given the name *Jacobi-Davidson* (**JD**) algorithm in [28]; a more detailed discussion on the relations with the methods of Davidson and Jacobi can be found in [28].
(b) THEOREM 3.14 indicates a relation to Shift-and-Invert Arnoldi (cf., e.g., [23,

ALG. 8.1]). For this algorithm the user has to provide a complex value μ and the algorithm locates the approximate eigenvalue nearest to μ with associated eigenvector. The algorithm is based on Arnoldi's method for $(\mathbf{A} - \mu\,\mathbf{I})^{-1}$. If we take in step (e) of ALGORITHM 2 for $\mathbf{z}_1$ the exact solution of the correction equation (in which ϑ is replaced by μ), then our search space $\mathcal{V}_k$ coincides with the Krylov subspace $\mathcal{K}_k((\mathbf{A} - \mu\,\mathbf{I})^{-1}; \mathbf{v}_1)$ (cf. TH. 3.14), i.e., the 'search space' of Shift-and-Invert Arnoldi. Therefore, if we orthogonalize in step (g) of ALGORITHM 2 against the previously constructed $\mathbf{V}$, then (except for some scalar multiple) the orthonormal basis vectors for both algorithms coincide and both algorithms produce the same approximate eigenpair. Since, Arnoldi's method exploits the Hessenberg structure of the projected matrix (here the projection of $(\mathbf{A} - \mu\,\mathbf{I})^{-1}$), Shift-and-Invert Arnoldi is more efficient than **JD** in this special case.

Replacing the 'target value' μ by the currently optimal approximate eigenvalue ϑ in Shift-and-Invert Arnoldi may be expected to lead to faster convergence but it affects also the efficiency: the projected matrix will be dense and in exact arithmetic both methods lead to the same results at the same costs. Since it may be expensive to work with $(\mathbf{A} - \vartheta\,\mathbf{I})^{-1}$ (i.e., to solve equations as $(\mathbf{A} - \vartheta\,\mathbf{I})\mathbf{z} = \mathbf{r}$ exactly) in each step, one might prefer suitable approximations $\mathbf{K}$ of $\mathbf{A} - \vartheta\,\mathbf{I}$ or of $\mathbf{A} - \mu\,\mathbf{I}$ (preconditioners; cf. [4, 7, 16, 17, 19]). Then, in **JD**, the search space is expanded by some appropriate linear combination of $\mathbf{K}^{-1}(\mathbf{A} - \vartheta\,\mathbf{I})\mathbf{u}$ and $\mathbf{K}^{-1}\mathbf{u}$ while the Shift-and-Invert Arnoldi, properly adapted, will expand by $\mathbf{K}^{-1}\mathbf{u}$ only. However, in view of the success of Davidson's method the component $\mathbf{K}^{-1}(\mathbf{A} - \vartheta\,\mathbf{I})\mathbf{u}$ is apparently important.

5. The search space and the test space. For the approximation of the eigenvector $\mathbf{x}$ in a relatively small number k of sweeps, we wish to construct a search space $\mathcal{V}_k$ that makes a (very) small angle with the vector $\mathbf{x}$. The choice $\mathcal{V}_k = \mathrm{span}(\mathbf{x})$ is optimal, but impractical. We will first consider the construction of suitable test spaces and after that we will consider the search space.

5.1. The test space. We will be interested in the non-trivial solutions $\mathbf{u}$, ϑ of the projected eigenproblem (26). The test space determines the way of projection, e.g., orthogonal with $\mathcal{W}_k = \mathcal{V}_k$, or oblique with other choices.

Different choices can be made for $\mathcal{W}_k$. Besides the choice for $\mathcal{W}_k$ as a space of approximating left eigenvectors (cf. Sect. 5.1.3), the following three other choices are obvious and allow for a familiar interpretation that we will discuss (in Sect. 5.1.1 and 5.1.2): $\mathcal{W}_k = \mathcal{V}_k$, $\mathcal{W}_k = \mathbf{A}\mathcal{V}_k$, and $\mathcal{W}_k = \mathbf{B}\mathcal{V}_k$.

These interpretations involve Ritz vectors and harmonic Ritz vectors:
if $\mathbf{A}$ is an $n \times n$ matrix and $\mathcal{V}$ is a k-dimensional subspace of $\mathbb{C}^k$ then a non-zero vector $\mathbf{u}$ in $\mathcal{V}$ and a scalar $\vartheta \in \mathbb{C}$ are called a *Ritz vector* and *Ritz value*, respectively, of $\mathbf{A}$ with respect to $\mathcal{V}$ if $\mathbf{A}\mathbf{u} - \vartheta\,\mathbf{u} \perp \mathcal{V}$. They are referred to as *harmonic Ritz vector* and *harmonic Ritz value*, respectively, of $\mathbf{A}$ with respect to $\mathcal{V}$ if $\mathbf{A}\mathbf{u} - \vartheta\,\mathbf{u} \perp \mathbf{A}\mathcal{V}$ [21, 28]. Note that $\mathbf{u}$ is a harmonic Ritz vector of $\mathbf{A}$ with respect to $\mathcal{V}$ if and only if $\mathbf{A}\mathbf{u}$ is a Ritz vector of $\mathbf{A}^{-1}$ with respect to the space $\mathbf{A}\mathcal{V}$.

In computations, sequences $(\mathcal{V}_k)$ of subspaces of increasing dimension are constructed, where the k-dimensional subspace $\mathcal{V}_k$ is a subset of the $k+1$ dimensional subspace $\mathcal{V}_{k+1}$. When $\mathbf{A}$ is normal (or close to normal) then the extremal Ritz values usually exhibit some regular convergence behavior towards extremal eigenvalues, while the in absolute smallest harmonic Ritz values usually show a regular convergence behavior towards the in absolute value smallest eigenvalues (for this property for symmetric matrices, see [21]). These properties may be used for the selection of the approximations of interest, especially for restarting purposes.

Once we have $\mathbf{V}_k$, any of the matrices $\mathbf{AV}_k$ and $\mathbf{BV}_k$ can easily be computed, and probably will be computed anyway to facilitate the computation of the $k \times k$ matrices $\mathbf{W}_k^*\mathbf{AV}_k$ and $\mathbf{W}_k^*\mathbf{BV}_k$.

In the next subsections we will discuss some choices for $\mathbf{W}$ for the important case that $\mathbf{B}$ is nonsingular.

5.1.1. B is non-singular.

(a) $\mathbf{W} = \mathbf{AV}$. The solutions of (26) with $\mathcal{W}_k = \mathbf{A}\mathcal{V}_k$ correspond to harmonic Ritz values of $\mathbf{AB}^{-1}$ with respect to the space $\widetilde{\mathbf{V}} := \mathbf{BV}$. That means that for $\widetilde{\mathbf{u}} = \mathbf{Bu}$ with $\mathbf{u} \in \mathbf{V}$ the requirement

$$\mathbf{AB}^{-1}\widetilde{\mathbf{u}} - \vartheta\,\widetilde{\mathbf{u}} \perp \mathbf{AB}^{-1}\widetilde{\mathbf{V}}$$

is equivalent to (26) with $\mathcal{W}_k = \mathbf{A}\mathcal{V}_k$.

(b) $\mathbf{W} = \mathbf{BV}$. The solution of (26) with $\mathcal{W}_k = \mathbf{B}\mathcal{V}_k$ corresponds to Ritz values of $\mathbf{AB}^{-1}$ with respect to the subspace $\widetilde{\mathbf{V}} := \mathbf{BV}$ in the following sense. For $\widetilde{\mathbf{u}} = \mathbf{Bu}$ with $\mathbf{u} \in \mathbf{V}$ we have that

$$\mathbf{AB}^{-1}\widetilde{\mathbf{u}} - \vartheta\,\widetilde{\mathbf{u}} \perp \widetilde{\mathbf{V}}$$

is equivalent to (26) with $\mathcal{W}_k = \mathbf{B}\mathcal{V}_k$.

5.1.2. B is positive definite. If $\mathbf{B}$ is positive definite then we can exploit a $\mathbf{B}$-inner product and associated orthogonality.

(a) $\mathbf{W} = \mathbf{V}$. The solutions of (26) with $\mathcal{W}_k = \mathcal{V}_k$ correspond to:
(a1) Ritz values of $\mathbf{AB}^{-1}$ with respect to the $\mathbf{B}^{-1}$-inner product and the subspace $\widetilde{\mathbf{V}} := \mathbf{BV}$, in the following way. For $\widetilde{\mathbf{u}} = \mathbf{Bu}$ with $\mathbf{u} \in \mathbf{V}$ it follows that

$$\mathbf{AB}^{-1}\widetilde{\mathbf{u}} - \vartheta\,\widetilde{\mathbf{u}} \perp_{\mathbf{B}^{-1}} \widetilde{\mathbf{V}}$$

is equivalent to (26) with $\mathcal{W}_k = \mathcal{V}_k$.
(a2) Ritz values of $\mathbf{B}^{-\frac{1}{2}}\mathbf{AB}^{-\frac{1}{2}}$ with respect to the subspace $\widetilde{\mathbf{V}} := \mathbf{B}^{\frac{1}{2}}\mathbf{V}$, as follows: for $\widetilde{\mathbf{u}} = \mathbf{B}^{\frac{1}{2}}\mathbf{u}$ with $\mathbf{u} \in \mathbf{V}$ we have that

$$\mathbf{B}^{-\frac{1}{2}}\mathbf{AB}^{-\frac{1}{2}}\widetilde{\mathbf{u}} - \vartheta\,\widetilde{\mathbf{u}} \perp \widetilde{\mathbf{V}}$$

is equivalent to (26) with $\mathcal{W}_k = \mathcal{V}_k$.

(b) $\mathbf{W} = \mathbf{AV}$. The solutions of (26) with $\mathcal{W}_k = \mathbf{A}\mathcal{V}_k$ correspond to harmonic Ritz values of $\mathbf{B}^{-\frac{1}{2}}\mathbf{AB}^{-\frac{1}{2}}$ with respect to the $\mathbf{B}$-inner product and the space $\widetilde{\mathbf{V}} := \mathbf{B}^{\frac{1}{2}}\mathbf{V}$ in the following way. For $\widetilde{\mathbf{u}} = \mathbf{B}^{\frac{1}{2}}\mathbf{u}$ with $\mathbf{u} \in \mathbf{V}$ we have that

$$\mathbf{B}^{-\frac{1}{2}}\mathbf{AB}^{-\frac{1}{2}}\widetilde{\mathbf{u}} - \vartheta\,\widetilde{\mathbf{u}} \perp_{\mathbf{B}} \mathbf{B}^{-\frac{1}{2}}\mathbf{AB}^{-\frac{1}{2}}\widetilde{\mathbf{V}}$$

is equivalent to (26) with $\mathcal{W}_k = \mathbf{A}\mathcal{V}_k$.

5.1.3. The test space as a search space. As explained in Section 3.2, we obtain fast convergence if the $\mathbf{w}$ converge to the left eigenvector. Therefore, the construction of $\mathcal{W}_k$ similar to $\mathcal{V}_k$ is straight forward: solve both the correction equation (11) and the adjoint correction equation (21) approximately (the Bi-CG method seems to fit quite naturally in this approach), and extend the search space and the test space by the computed corrections. Then take $\mathbf{w} = \mathbf{W}_k y$, where y is the left eigenvector of the projected eigenproblem associated with ϑ.

5.2. On the choice of w. We have discussed choices for $\mathbf{w}$, $\widetilde{\mathbf{w}}$ and $\widetilde{\mathbf{u}}$ in Section 3. However, these choices can not be completely independent from the spaces $\mathcal{V}_k$ and $\mathcal{W}_k$. For instance, $\mathbf{w}$ should be in $\mathcal{W}_k$, and should not be orthogonal to $\widetilde{\mathbf{w}}$.

For a number of choices (cf. Sect. 3.3), $\mathbf{w}$ should not be orthogonal to $\mathbf{u}$ as well. In particular, $\mathbf{u}$ should not be orthogonal to $\mathcal{W}_k$ and it is quite natural to require that the spaces $\mathcal{V}_k$ and $\mathcal{W}_k$ are not mutually orthogonal.

If $\mathbf{W} = \mathbf{BV}$, then the choices $\widetilde{\mathbf{w}} = \mathbf{w} = \mathbf{Bu}$ and $\widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{w}$ are obvious. The same remark applies to the combination of $\mathbf{W} = \mathbf{AV}$, $\widetilde{\mathbf{w}} = \mathbf{w} = \mathbf{Au}$, and $\widetilde{\mathbf{u}} = \mathbf{A}^*\mathbf{w}$.

Also if the test space $\mathcal{W}_k$ is not constructed as to approach a subspace of left eigenvectors (cf. Sect. 5.1.3) then still the use of left eigenvectors may help to improve the convergence: select $\mathbf{w} = \mathbf{W}_k y_\ell$, where y_ℓ is the left eigenvector of the projected problem.

5.3. The basis of the search space and its test space. For stability reasons the basis of the search space as well as of the test space should satisfy certain orthogonality properties.

For instance, $\mathbf{v}_{k+1} := \mathbf{v}'/\|\mathbf{v}'\|$, with $\mathbf{v}' := \mathbf{z}_1 - \mathbf{V}_k\mathbf{V}_k^*\mathbf{z}_1$, leads to an orthonormal basis for the search space and $\mathbf{V}_k^*\mathbf{V}_k = I$. Of course, the vector $\mathbf{v}'$ can also be computed by modified Gram-Schmidt. For accuracy reasons, this modified approach is even to be preferred.

If $\mathbf{B}$ is positive definite, then $\mathbf{v}_{k+1} := \mathbf{v}'/\gamma$ with $\mathbf{v}' := \mathbf{z}_1 - \mathbf{V}_k\mathbf{V}_k^*\mathbf{B}\mathbf{z}_1$ and $\gamma^2 := \mathbf{v}'^*\mathbf{B}\mathbf{v}'$, leads to a $\mathbf{B}$-orthonormal basis: $\mathbf{V}_k^*\mathbf{B}\mathbf{V}_k = I$ which simplifies the projected problem to $\mathbf{V}_k^*\mathbf{A}\mathbf{V}_k - \vartheta I$ if $\mathcal{W}_k = \mathcal{V}_k$.

Assume that $\mathcal{W}_k = \mathbf{B}\mathcal{V}_k$ is the selected test space. Then $\mathbf{w}_{k+1} := \mathbf{w}'/\|\mathbf{w}'\|$, $\mathbf{v}_{k+1} := \mathbf{v}'/\|\mathbf{w}'\|$. with $\mathbf{w}' := \mathbf{B}\mathbf{z}_1 - \mathbf{W}_k\mathbf{W}_k^*\mathbf{B}\mathbf{z}_1$ and $\mathbf{v}' := \mathbf{z}_1 - \mathbf{V}_k\mathbf{W}_k^*\mathbf{B}\mathbf{z}_1$, leads to an orthonormal basis for the subspace $\mathcal{W}_k$: $\mathbf{W}_k^*\mathbf{W}_k = I$, while $\mathbf{B}\mathbf{V}_k = \mathbf{W}_k$. The projected problem reduces in this case to $\mathbf{W}_k^*\mathbf{A}\mathbf{V}_k - \vartheta I$.

6. The solution of the projected eigenproblem. The projected eigenproblem (27) is a relatively small eigenproblem of dimension $\dim(\mathrm{span}(\mathbf{V}_k))$ and can be solved relative efficiently by standard algorithms such as the QR-algorithm. Of course, if one is interested in, for instance, only the eigenvalue with largest real part, then there is no need to compute all eigenvalues of the projected problem. However, if one is interested in a interior eigenvalue, then it may be helpful to compute all Petrov-Ritz values: this may facilitate the selection of the appropriate approximating eigenvalue.

The computation of the projected matrix, e.g., $\mathbf{W}_k^*\mathbf{A}\mathbf{V}_k$ involves the evaluation of a number of inner products. Using the fact that

$$\mathbf{W}_{k+1}^*\mathbf{A}\mathbf{V}_{k+1} = \begin{bmatrix} \mathbf{W}_k^*\mathbf{A}\mathbf{V}_k & \mathbf{W}_k^*\mathbf{A}\mathbf{v}_{k+1} \\ \mathbf{w}_{k+1}^*\mathbf{A}\mathbf{V}_k & \mathbf{w}_{k+1}^*\mathbf{A}\mathbf{v}_{k+1} \end{bmatrix},$$

if $\mathbf{V}_{k+1} = [\mathbf{V}_k, \mathbf{v}_{k+1}]$, $\mathbf{W}_{k+1} = [\mathbf{W}_k, \mathbf{w}_{k+1}]$, reduces the number of inner products per sweep.

7. The correction equation. We will have an accurate approximation for the eigenvector $\mathbf{x}$ if the angle between $\mathbf{x}$ and the search space $\mathcal{V}_k$ is sufficiently small. We can achieve small angles in two ways: by building high dimensional search spaces $\mathcal{V}_k$ (k large), or by carefully selecting the vectors $\mathbf{z}_1$ by which we extend these subspaces $\mathcal{V}_k$. To make this more precise, we extend $\mathcal{V}_k$ by $\mathbf{z}_1$, where $\mathbf{z}_1$ is an approximate solution of

(a) the correction equation (11) or of
(b) the complete set of eigenvalue equations (9).

More accurate solutions of (9) will involve more computational work in terms of matrix vector multiplications for the solution of part (9)(b), while for (11) the higher dimensional subspaces $\mathcal{V}_k$ require more vector updates in the steps where the matrices are projected onto $\mathcal{V}_k$ and for the construction of the Ritz vector. We have the alternative of inexpensive inner loops (where the corrections equation is solved) in combination with more expensive outer loops (where the projected eigenproblem is solved) and expensive inner loops with inexpensive outer loops. The optimal strategy will depend on the convergence properties and on costs of a matrix-vector product as compared with vector updates.

For local efficiency reasons one may prefer more accurate solutions of (9). However, since the quadratic convergence of the **JD** process will only occur for larger k (the convergence is asymptotically quadratic), one may postpone the fast convergence by investing the computational effort in obtaining accurate solutions of (9) rather than building larger search spaces $\mathcal{V}_k$. For instance, if one uses Newton's process for the solution of (9), then one may see a very slowly converging or even a diverging process if the initial guess (computed from results in the outer loop) is not accurate enough.

There are a number of ways to achieve efficiently more accurate solutions of (9) with iterative methods. One may think of

(a) preconditioning (cf. Sect. 7.1),
(b) using the subspace, that was constructed to solve (11) approximately, in order to obtain an approximate solution of (9),
(c) using the subspace that has been constructed in the outer loop, in order to obtain a more accurate approximation of (11),
(d) iterating (9), say, ℓ times ($\ell \geq 2$) by the Jacobi correction method (as described in the paragraph following (3)),
(e) iterating (9), say, ℓ times with Newton process (cf. Sect. 7.2), or
(f) combinations of these strategies.

If one uses ℓ steps of some iterative process to solve (9), as in (d) or (e), then there will be an optimal ℓ as far as the overall efficiency is concerned.

In the next subsections we will discuss the option of preconditioning and the use of Newton's method, the other possibilities will be subject of further study.

7.1. Preconditioning. If $\mathbf{M}_p$ is an approximation for the inverse of the projected matrix $\mathbf{F}_p$ in (12), then one may use this operator in order to get an accurate solution $\mathbf{z}$ of the correction equation (11) in fewer iteration steps. The preconditioner should map the image space $\mathbf{w}^\perp$ of $\mathbf{F}_p$ onto its domain space $\widetilde{\mathbf{u}}^\perp$. Therefore, $\mathbf{M}_p$

should satisfy

$$\mathbf{M}_p = \left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right) \mathbf{M}_p \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right). \tag{28}$$

Then the preconditioned correction equation for $\mathbf{z} \perp \widetilde{\mathbf{u}}$ reads as

$$\mathbf{M}_p\,\mathbf{F}_p\,\mathbf{z} = \mathbf{M}_p(\mathbf{A} - \vartheta\,\mathbf{B}) \left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right) \mathbf{z} = -\mathbf{M}_p\,\mathbf{r}. \tag{29}$$

Here we exploit the fact that projections are involved: applying such a map once has the same effect as applying it twice. In the context of Krylov subspace methods, the following similar observation is useful:

$$\mathbf{M}_p\,\mathbf{F}_p\,\mathbf{y} = \mathbf{M}_p(\mathbf{A} - \vartheta\,\mathbf{B})\,\mathbf{y} \quad \text{if} \quad \mathbf{y} = \mathbf{M}_p\,\widetilde{\mathbf{y}},$$

since the vectors involved in the iteration process usually can be written in the latter form.

7.1.1. Projecting preconditioners. In most cases, preconditioners are specified as approximations $\mathbf{K}$ for $\mathbf{A} - \vartheta\,\mathbf{B}$, and such that the equation $\mathbf{K}\mathbf{t} = \mathbf{r}$ can be solved relatively easily. For instance, Davidson [6] suggested $\mathbf{K} = \mathrm{diag}(\mathbf{A}) - \vartheta\,\mathrm{diag}(\mathbf{B})$ (see also [18, 7]). In view of our observations in Section 3 we expect to create better preconditioners by taking the projections into account. Therefore, we consider the inverse as a map from $\widetilde{\mathbf{u}}^\perp$ onto $\mathbf{w}^\perp$ of $\mathbf{K}_p$, the projection of $\mathbf{K}$,

$$\mathbf{K}_p := \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right) \mathbf{K} \left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right). \tag{30}$$

The following propositions (PROP. 7.1, 7.3 and 7.6) express the inverse of $\mathbf{K}_p$ in terms of the inverse of $\mathbf{K}$. The operator $\mathbf{K}_p^{-1}$ denotes the inverse of $\mathbf{K}_p$ as a map from $\widetilde{\mathbf{u}}^\perp$ onto $\mathbf{w}^\perp$.

PROPOSITION 7.1. *If* $\mathbf{K}$ *maps* $\widetilde{\mathbf{u}}^\perp$ *onto* $\mathbf{w}^\perp$ *then* $\mathbf{K}_p^{-1}$ *exists with respect to the subspace* $\mathbf{w}^\perp$*, and*

$$\mathbf{K}_p^{-1} = \left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right) \mathbf{K}^{-1} \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right) = \mathbf{K}^{-1}. \tag{31}$$

Proof. If $\mathbf{y} \perp \mathbf{w}$ and $\mathbf{t}$ is such that $\mathbf{K}\mathbf{t} = \mathbf{y}$ then $\mathbf{t} \perp \widetilde{\mathbf{u}}$ and $\mathbf{K}_p\mathbf{t} = \mathbf{y}$. □

REMARK 7.2. The condition in PROPOSITION 7.1 is satisfied if, for instance, $\mathbf{K}$ is diagonal and if $\mathbf{w} = \widetilde{\mathbf{u}}$ is a standard basis vector. Then, for any $\mathbf{y} \perp \mathbf{w}$, we can compute $\mathbf{K}_p^{-1}\mathbf{y}$ without projection: $\mathbf{K}_p^{-1}\mathbf{y} = \mathbf{K}^{-1}\mathbf{y}$.

In general, for non-diagonal preconditioners, the projections can not be ignored, that is skipping the projections may lead to slower convergence. For a numerical example, see [31]. For this general situation, it is not so obvious how to compute $\mathbf{K}_p$, and the following proposition may be helpful.

PROPOSITION 7.3. *If* $\mathbf{K}$ *is non-singular and* $\widetilde{\mathbf{u}}^*\mathbf{K}^{-1}\widetilde{\mathbf{w}} \neq 0$ *then* $\mathbf{K}_p^{-1}$ *exists with respect to the subspace* $\mathbf{w}^\perp$*, and*

$$\mathbf{K}_p^{-1} = \mathbf{K}^{-1}\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{y}_r^*}{\mathbf{y}_r^*\widetilde{\mathbf{w}}}\right) = \left(\mathbf{I} - \frac{\mathbf{y}_\ell\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{y}_\ell}\right) \mathbf{K}^{-1}, \tag{32}$$

where $\mathbf{y}_r$ *solves* $\mathbf{K}^*\mathbf{y}_r = \widetilde{\mathbf{u}}$ *and* $\mathbf{y}_\ell$ *solves* $\mathbf{K}\mathbf{y}_\ell = \widetilde{\mathbf{w}}$.

Proof. Observe that $\widetilde{\mathbf{u}}^*\mathbf{y}_\ell = \mathbf{y}_r^*\widetilde{\mathbf{w}} \neq 0$. Clearly the second equality holds.

If $\mathbf{K}\mathbf{t} = \mathbf{r} + \beta\widetilde{\mathbf{w}}$ with scalar β such that $\widetilde{\mathbf{u}} \perp \mathbf{t}$ then $\mathbf{K}_p\mathbf{t} = \mathbf{r}$, leading to the first equality in (32). □

THEOREM 7.4. *If* $\mathbf{K}$ *is non-singular and* $\widetilde{\mathbf{u}}^*\mathbf{K}^{-1}\widetilde{\mathbf{w}} \neq 0$ *then the correction equation* (11) *preconditioned by* $\mathbf{K}_p^{-1}$ *(cf.* PROP. 7.3*) is equivalent to*

$$\mathbf{z} \perp \widetilde{\mathbf{u}} \quad \textit{and} \quad \left(\mathbf{I} - \frac{\mathbf{y}_\ell\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{y}_\ell}\right)\mathbf{K}^{-1}(\mathbf{A} - \vartheta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{y}_\ell\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{y}_\ell}\right)\mathbf{z} = -\mathbf{r}', \tag{33}$$

where

$$\mathbf{y}_\ell := \mathbf{K}^{-1}\widetilde{\mathbf{w}} \quad \textit{and} \quad \mathbf{r}' := \left(\mathbf{I} - \frac{\mathbf{y}_\ell\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{y}_\ell}\right)\mathbf{K}^{-1}\mathbf{r}. \tag{34}$$

Proof. Since, with $\mathbf{y}_r$ as in PROPOSITION 7.3,

$$\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{y}_r^*}{\mathbf{y}_r^*\widetilde{\mathbf{w}}}\right)\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right) = \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{y}_r^*}{\mathbf{y}_r^*\widetilde{\mathbf{w}}}\right),$$

equation (32) shows that the preconditioned correction equation is equivalent to

$$\mathbf{z} \perp \widetilde{\mathbf{u}} \quad \text{and} \quad \left(\mathbf{I} - \frac{\mathbf{y}_\ell\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{y}_\ell}\right)\mathbf{K}^{-1}(\mathbf{A} - \vartheta\,\mathbf{B})\left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}', \tag{35}$$

with $\mathbf{y}_\ell$ and $\mathbf{r}'$ as in (34). Finally, the equivalence of (33) and (35) follows from the fact that

$$\mathbf{z} \perp \widetilde{\mathbf{u}} \quad \Leftrightarrow \quad \mathbf{z} = \left(\mathbf{I} - \frac{\mathbf{y}_\ell\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{y}_\ell}\right)\mathbf{z} \quad \Leftrightarrow \quad \mathbf{z} = \left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z}.$$

□

In [31] a diagonal block approximation $\mathbf{K}$ of $\mathbf{A} - \vartheta\,\mathbf{B}$, in combination with a block approximation of the projections using the same block structure, was reported to be successful.

REMARK 7.5. In the Davidson methods [4, 6, 17, 18] the search space is expanded by the vector $\mathbf{K}^{-1}\mathbf{r}$, the vector that appears in the first step of the computation of $\mathbf{r}'$ (cf. TH. 7.4). In Olsen's method (cf. [20]), for symmetric eigenproblems with $\widetilde{\mathbf{u}} = \widetilde{\mathbf{w}} = \mathbf{u}$, the search space is expanded by the vector $\mathbf{r}'$ (see also [28]).

If $\mathbf{K}$ is a good approximation of $\mathbf{A} - \lambda\,\mathbf{B}$ then $\mathbf{K}$ may be non-singular and the following proposition may be useful[1].

PROPOSITION 7.6. *If* $\mathrm{Ker}(\mathbf{K}) = \mathrm{span}(\mathbf{a})$ *for some non-trivial vector* $\mathbf{a}$ *then there is a non-trivial vector* $\mathbf{b}$ *for which* $\mathrm{Ker}(\mathbf{K}^*) = \mathrm{span}(\mathbf{b})$ *and*

$$\mathbf{K}_p^{-1} = \left(\mathbf{I} - \frac{\mathbf{a}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{a}}\right)\mathbf{K}^{-1}\left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{b}^*}{\mathbf{b}^*\widetilde{\mathbf{w}}}\right) \quad \textit{on} \quad \mathbf{w}^\perp, \tag{36}$$

where $\mathbf{K}^{-1}$ *is the inverse of* $\mathbf{K}$ *as a map from* $\mathbf{a}^\perp$ *onto* $\mathbf{b}^\perp$.

Proof. If $\mathbf{K}\mathbf{t} = \mathbf{K}(\mathbf{t} + \alpha\mathbf{a}) = \mathbf{r} + \beta\widetilde{\mathbf{w}}$ with scalars α and β such that $\mathbf{b} \perp \mathbf{r} + \beta\widetilde{\mathbf{w}}$ and $\widetilde{\mathbf{u}} \perp \mathbf{t} + \alpha\mathbf{a}$ then $\mathbf{K}_p\mathbf{t} = \mathbf{r}$. This leads to (36). □

[1] The idea exposed in the proposition was also suggested by Dr. F. Wubs (private communication)

7.1.2. The augmented correction equation. Formulation (23) of the correction equation (11) (for the case $\mathbf{r} \perp \mathbf{w}$) may be more accessible for the construction of suitable preconditioners, avoiding explicit projections as in Section 7.1.1.

The following lemma, for which we omit the obvious proof, is helpful for the construction inverses corresponding to equation (23).

LEMMA 7.7. *For* $\mathbf{z}$ *and* $\mathbf{y}$ *we have*

$$\begin{bmatrix} \mathbf{I} & \mathbf{y} \\ \mathbf{z}^* & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{I} & 0 \\ \mathbf{z}^* & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} & \mathbf{y} \\ 0^* & -\nu \end{bmatrix} \quad \textit{where} \quad \nu := \mathbf{z}^*\mathbf{y},$$

and the matrix is invertible if and only if $\mathbf{z}^*\mathbf{y} \neq 0$.

If $\mathbf{K}$ is an easily invertible approximation of $\mathbf{A} - \vartheta\,\mathbf{B}$ then the augmented equation (23) can be preconditioned by

$$\begin{bmatrix} \mathbf{K} & \widetilde{\mathbf{w}} \\ \widetilde{\mathbf{u}}^* & 0 \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{I} & -\mathbf{y}_\ell \\ 0^* & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 \\ \frac{\widetilde{\mathbf{u}}^*}{\nu} & \frac{-1}{\nu} \end{bmatrix} \begin{bmatrix} \mathbf{K}^{-1} & 0 \\ 0^* & 1 \end{bmatrix}, \quad \text{where} \quad \begin{cases} \mathbf{y}_\ell := \mathbf{K}^{-1}\widetilde{\mathbf{w}} \\ \nu := \widetilde{\mathbf{u}}^*\mathbf{y}_\ell. \end{cases} \tag{37}$$

and

$$\begin{bmatrix} \mathbf{K} & \widetilde{\mathbf{w}} \\ \widetilde{\mathbf{u}}^* & 0 \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{A} - \vartheta\,\mathbf{B} & \widetilde{\mathbf{w}} \\ \widetilde{\mathbf{u}}^* & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{I} & -\mathbf{y}_\ell \\ 0^* & 1 \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 \\ \frac{\widetilde{\mathbf{u}}^*}{\nu} & \frac{-1}{\nu} \end{bmatrix} \begin{bmatrix} \mathbf{K}^{-1}(\mathbf{A} - \vartheta\,\mathbf{B}) & \mathbf{y}_\ell \\ \widetilde{\mathbf{u}}^* & 0 \end{bmatrix}. \tag{38}$$

For more efficient computation, we prefer the factorized form at the right hand sides of equations (37) and (38).

Clearly (37) has also a 'left variant' (with $\mathbf{K}^{-1}$ at the left in the right hand side). The left variant may be more suitable for post preconditioning of the augmented equation (23). Both variants are obvious analogues of the preconditioners in (32); likewise, (38) is an analogue of (33).

EXAMPLES 7.8. By taking $\widetilde{\mathbf{w}} = (\lambda - \mu)\mathbf{B}\mathbf{u}$, and $\widetilde{\mathbf{u}}$ and $\mathbf{u}$ scaled such that $\widetilde{\mathbf{u}}^*\mathbf{u} = 1$, then the choice $\mathbf{K} = \mathbf{A} - \mu\mathbf{B}$ leads to $\mathbf{y}_\ell = \mathbf{u} - (\vartheta - \lambda)\mathbf{K}^{-1}\mathbf{B}\mathbf{u} - \mathbf{K}^{-1}\mathbf{r}$. Then $\mathbf{y}_\ell \approx \mathbf{u}$ and $\nu = \widetilde{\mathbf{u}}^*\mathbf{y}_\ell \approx \widetilde{\mathbf{u}}^*\mathbf{u} = 1$ if $\mathbf{r} \approx 0$, suggesting a way to save one matrix-vector multiplication (in the computation of $\mathbf{y}_\ell$ in (37) and (38)): take the right hand sides of (37) and (38), and replace ν by 1 and $\mathbf{y}_\ell$ by $\mathbf{u}$. Note that the unknown scalar λ does not appear in the correction equation that is preconditioned as described here. For the suggested choice of $\mathbf{K}$, the equation $\mathbf{K}\mathbf{t} = \mathbf{z}$ can efficiently be solved if, for instance, an LU-decomposition of $\mathbf{K}$ is available. We emphasize that, in this approach, the L and U factors have to be computed only once: that is, we suggest not to update $\mathbf{K}$ when we have an approximation ϑ closer to λ than μ.

7.2. Newton's method. Before demonstrating how Newton's method leads to an iterative scheme for the solution of (3), we will discuss this method for the more fundamental equation $r(\widetilde{\mathbf{u}}) = 0$ with r as defined in (39) below. However, the two approaches will turn out to be equivalent.

Eigenvectors with scaled component. First select two vectors $\mathbf{w}$ and $\widetilde{\mathbf{u}}$. We concentrate on the computation of the eigenvectors $\mathbf{x}$ that have a normalized component in the direction of $\widetilde{\mathbf{u}}$: $(\mathbf{x}, \widetilde{\mathbf{u}}) = 1$.
Consider the map r from the $(n-1)$-dimensional hyperplane $\{\, \mathbf{y} \in \mathbb{C}^n \mid (\mathbf{y}, \widetilde{\mathbf{u}}) = 1\}$ to the $(n-1)$-dimensional subspace $\{\, \mathbf{y} \in \mathbb{C}^n \mid (\mathbf{y}, \mathbf{w}) = 0\}$ define by

$$r(\mathbf{u}) := \mathbf{A}\mathbf{u} - \vartheta(\mathbf{u})\,\mathbf{B}\mathbf{u} \quad \text{where} \quad \vartheta(\mathbf{u}) := \frac{\mathbf{w}^*\mathbf{A}\mathbf{u}}{\mathbf{w}^*\mathbf{B}\mathbf{u}} \qquad \forall\, \mathbf{u},\ (\mathbf{u}, \widetilde{\mathbf{u}}) = 1. \tag{39}$$

The Newton process for zeros of r produces a sequence $\mathbf{u}_k$ such that

$$\mathbf{u}_{k+1} = \mathbf{u}_k - \mathbf{f}_k \quad \text{with} \quad \mathbf{f}_k \perp \widetilde{\mathbf{u}},$$

where the correction $\mathbf{f}_k$ is the solution of the residual equation involving the Jacobian Dr of r:

$$Dr_{|\mathbf{u}_k}(\mathbf{f}_k) = \mathbf{r}_k := r(\mathbf{u}_k) = \mathbf{A}\mathbf{u}_k - \vartheta_k \mathbf{B}\mathbf{u}_k \quad \text{with} \quad \vartheta_k := \vartheta(\mathbf{u}_k).$$

Since

$$\vartheta'_{|\mathbf{u}}(\mathbf{f}) = \frac{\mathbf{w}^*(\mathbf{A} - \vartheta(\mathbf{u})\,\mathbf{B})\mathbf{f}}{\mathbf{w}^*\mathbf{B}\mathbf{u}} \quad \text{and} \quad Dr_{|\mathbf{u}}(\mathbf{f}) = -\vartheta'_{|\mathbf{u}}(\mathbf{f})\,\mathbf{B}\mathbf{u} + (\mathbf{A} - \vartheta(\mathbf{u})\,\mathbf{B})\mathbf{f},$$

we see that

$$Dr_{|\mathbf{u}}(\mathbf{f}) = \left(\mathbf{I} - \frac{\mathbf{B}\mathbf{u}\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{u}}\right)(\mathbf{A} - \vartheta(\mathbf{u})\,\mathbf{B})\,\mathbf{f}$$

and the correction equation for Newton reads as

$$\mathbf{f}_k \perp \widetilde{\mathbf{u}} \quad \text{and} \quad \left(\mathbf{I} - \frac{\mathbf{B}\mathbf{u}_k\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{u}_k}\right)(\mathbf{A} - \vartheta_k\mathbf{B})\;\mathbf{f}_k = \mathbf{r}_k. \tag{40}$$

Note that the definition of $\vartheta(\mathbf{u})$ implies that $\mathbf{r}_k \perp \mathbf{w}$. Consequently, the projection in the left hand side does not affect $\mathbf{r}_k$.

Newton and the correction equation. Substitution of (3)(a) into the second one, leads to an expression for the correction $\mathbf{z} \perp \mathbf{u}$. Obviously, we can try to find an accurate solution of this equation by Newton's method.

Assume that we have an approximate solution $\mathbf{z} = \mathbf{z}_k$, with $\mathbf{z}_0 = 0$, (that is, a correction of the approximation $\mathbf{u}$ of the eigenvector). Then the Newton correction $\mathbf{f} = \mathbf{f}_k$ (of the approximate solution $\mathbf{z}_k$) is orthogonal to $\mathbf{u}$ and satisfies

$$\mathbf{f} \perp \mathbf{u} \quad \text{and} \quad (\mathbf{I} - \mathbf{Q})\,(\mathbf{I} - \mathbf{P})\,(\mathbf{A} - \vartheta_k\mathbf{B})\,\mathbf{f} = (\mathbf{I} - \mathbf{Q})\,(\mathbf{A} - \vartheta_k\mathbf{B})\,\mathbf{u}_k \tag{41}$$

where $\mathbf{u}_k := \mathbf{u} + \mathbf{z}_k$ and $\vartheta_k := \vartheta(\mathbf{u}_k)$ and the projections $\mathbf{P}$ and $\mathbf{Q}$ are given by

$$\mathbf{Q} := \frac{\mathbf{u}\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{u}} \quad \text{and} \quad \mathbf{P} := \frac{\mathbf{B}\mathbf{u}_k\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{u}_k}.$$

Since $\mathbf{Q}\mathbf{P} = \mathbf{Q}$ and $\mathbf{P}\mathbf{Q} = \mathbf{P}$ we have that $(\mathbf{I} - \mathbf{Q})(\mathbf{I} - \mathbf{P}) = (\mathbf{I} - \mathbf{P})$. Apparently, in exact arithmetic, (40) is equivalent to (41) (where, now, $\mathbf{u}$ is the $\widetilde{\mathbf{u}}$ of (40)).

In terms of projections, our observation in the last phrase of the previous subsection reads as $(\mathbf{I} - \mathbf{Q}) = (\mathbf{I} - \mathbf{P})(\mathbf{I} - \mathbf{Q})$.

Apparently, the effect of ℓ steps with Newton for (3) is an ℓ step iteration for (11), with appropriate choices of $\mathbf{w}$, $\widetilde{\mathbf{u}}$, $\widetilde{\mathbf{w}}$, and with updated approximations, or, loosely speaking, it is an ℓ-step **JD** without the intermediate 1-dimensional extensions of the approximating subspace $\mathcal{V}_k$.

8. Polynomial eigenvalue equations. For $\ell \in \mathbb{N}$, and $n \times n$ matrices $\mathbf{A}_0, \ldots, \mathbf{A}_\ell$, consider the generalized eigenproblem of finding an eigenvector $\mathbf{x}$ (non-trivial) and associated eigenvalue $\lambda \in \mathbb{C}$ such that

$$\mathbf{A}_0\mathbf{x} + \lambda\,\mathbf{A}_1\mathbf{x} + \cdots + \lambda^\ell \mathbf{A}_\ell \mathbf{x} = 0. \tag{42}$$

In terms of a matrix-valued polynomial $\mathbf{\Psi}$, we are interested in pairs $(\lambda, \mathbf{x})$ of scalars λ and non-trivial vectors $\mathbf{x}$ for which

$$\mathbf{\Psi}(\lambda)\,\mathbf{x} = 0 \quad \text{where} \quad \mathbf{\Psi}(\zeta) := \mathbf{A}_0 + \zeta\mathbf{A}_1 + \cdots + \zeta^\ell \mathbf{A}_\ell \quad (\zeta \in \mathbb{C}). \tag{43}$$

To solve this problem, we can proceed as before. Suppose we have a k-dimensional search space $\mathcal{V}_k$ and a k-dimensional projection space $\mathcal{W}_k$. Then, we can compute an approximation $\mathbf{u}$ of $\mathbf{x}$ with associated approximation ϑ of λ, by solving the projected problem:

$$\mathbf{u} \in \mathcal{V}_k, \;\; \vartheta \in \mathbb{C} \quad \text{such that} \quad \mathbf{\Psi}(\vartheta)\,\mathbf{u} \perp \mathcal{W}_k. \tag{44}$$

We define the residual $\mathbf{r}$ by

$$\mathbf{r} := \mathbf{\Psi}(\vartheta)\,\mathbf{u}, \tag{45}$$

and, for a some $\widetilde{\mathbf{u}}$, we correct the approximation $\mathbf{u}$ by $\mathbf{z}_1$, where $\mathbf{z}_1 \perp \widetilde{\mathbf{u}}$ is an approximate solution of the correction equation:

$$\mathbf{z} \perp \widetilde{\mathbf{u}} \quad \text{and} \quad \left(\mathbf{I} - \frac{\widetilde{\mathbf{w}}\,\mathbf{w}^*}{\mathbf{w}^*\widetilde{\mathbf{w}}}\right)\mathbf{\Psi}(\vartheta)\left(\mathbf{I} - \frac{\mathbf{u}\,\widetilde{\mathbf{u}}^*}{\widetilde{\mathbf{u}}^*\mathbf{u}}\right)\mathbf{z} = -\mathbf{r}, \tag{46}$$

for relevant choices of $\mathbf{w}$ and $\widetilde{\mathbf{w}}$, with $\mathbf{w}$ orthogonal to $\mathbf{r}$. As before, the approximate correction $\mathbf{z}_1$ can be used to extend the search space $\mathcal{V}_k$. By choosing basis in $\mathcal{V}_k$ and in $\mathcal{W}_k$, the projected problem (44) is equivalent to a small eigenproblem involving a $k \times k$-matrix-valued polynomial. If the sequences of $\mathbf{u}$, $\mathbf{w}$ and $\widetilde{\mathbf{u}}$ converge then, the choice

$$\widetilde{\mathbf{w}} := \mathbf{\Psi}'(\vartheta)\,\mathbf{u} = (\mathbf{A}_1 + 2\,\vartheta\mathbf{A}_2 + \cdots + \ell\,\vartheta^{\ell-1}\mathbf{A}_\ell)\,\mathbf{u} \tag{47}$$

leads to asymptotic quadratic convergence.

Recently, this approach with $\mathbf{w} = \widetilde{\mathbf{u}} = \mathbf{u}$ has been used successfully for the solution of quadratic eigenvalue problems associated with acoustic models [22].

9. Numerical examples.
In this section we will present some numerical examples.
These examples have been coded in Fortran. The small projected eigenvalue problem is solved with the Householder-QR (or QZ) algorithm [12], with routines from the LAPACK library [1]. With this algorithm we computed also the complete spectra of the matrix pairs in the examples, and we refer to these results as true (or correct) eigenvalues.

First, in Section 9.1, we illustrate the effect of specific choices for $\widetilde{\mathbf{w}}$, $\mathbf{w}$ and $\widetilde{\mathbf{u}}$ on the speed of convergence of **JD**. Then, in Section 9.2 we give some examples of the performance of **JD**, where $\mathbf{V}$ is $\mathbf{B}$-orthogonal and $\mathbf{V} = \mathbf{W}$, comparing this version of **JD** applied to the generalized eigenproblem with a naive version where **JD** is applied to the standard eigenproblem $\mathbf{B}^{-1}\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$. In Section 9.3, we discuss the effect of augmenting or projecting the preconditioner. There is a trade-off between the computational work, needed to solve the correction equation accurately enough, and the speed of convergence of **JD**. This issue will be discussed in Section 9.4. We also consider the performance of a block version (see Sect. 9.5).

9.1. The effect of the projections on the speed of convergence. In the previous sections various choices for the subspaces $\mathcal{V}_k$ and $\mathcal{W}_k$, and the vectors $\widetilde{\mathbf{w}}$, $\mathbf{w}$ and $\widetilde{\mathbf{u}}$ are discussed. Their implication for the speed of convergence is analyzed and it is shown theoretically that some of these choices lead to quadratic or even cubic convergence, while other choices only lead to linear or superlinear convergence. The purpose of this subsection is to illustrate by numerical examples our findings on the convergence speed.

We present some numerical results obtained for a generalized eigenvalue problem $\mathbf{Ax} = \lambda\mathbf{Bx}$ taken from the "Test Matrix Collection" [2], namely the Bounded Fineline Dielectric Waveguide problem of order 398. This problem stems from a finite element discretization of the Maxwell equation for propagating modes and magnetic field profiles of a rectangular waveguide filled with dielectric and PEC structures. The resulting matrix $\mathbf{A}$ is non-symmetric and the matrix $\mathbf{B}$ is positive definite. Both matrices are real (but may be complex in realistic applications). Of special interest are the eigenvalues with positive real part and their corresponding eigenvectors.

The correction equations (11) are (approximately) solved by (at most) 10 steps of GMRES, left preconditioned with an Incomplete LU(2) factorization of $\mathbf{A} - \tau\mathbf{B}$, for $\tau = 2500$. This had the effect that the correction equations were solved with a relative residual norm reduction of 10^{-9} as soon as the relative residual norm of the selected Petrov-Ritz pair became smaller than 10^{-2}. We choose the starting vectors $\mathbf{v} = \mathbf{v}_0$ and $\mathbf{w} = \mathbf{w}_0$ for the first sweep both equal to the vector with all ones scaled to unit length.

The selected Petrov-Ritz pair, was the one with the Petrov-Ritz value closest to τ and the iterations were stopped as soon as the relative residual norm for the Petrov-Ritz vector was smaller than 10^{-9}.

Since the 5 rightmost eigenvalues of this problem are (to 5 digits of accuracy):

$$\begin{aligned} \lambda_1 &= +2.9483e03, \\ \lambda_2 &= +4.0338e02, \\ \lambda_3 &= -1.0082e03, \\ \lambda_4 &= -1.5907e03, \\ \lambda_5 &= -2.0820e03. \end{aligned}$$

our choice of τ leads to convergence of the Petrov-Ritz pair to the largest eigenvalue λ_1.

Linear versus quadratic. We start with considering the following choices for $\widetilde{\mathbf{w}}$, $\mathbf{w}$ and $\widetilde{\mathbf{u}}$:

1. $\widetilde{\mathbf{w}} = \mathbf{w} = \widetilde{\mathbf{u}} = \mathbf{u}$, expecting linear convergence (cf. TH. 3.9),
2. $\widetilde{\mathbf{w}} = \mathbf{Bu}, \widetilde{\mathbf{u}} = \mathbf{w} = \mathbf{u}$, expecting quadratic convergence (cf. Sect. 3.1), and
3. $\widetilde{\mathbf{w}} = \mathbf{Bu}, \widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{u}, \mathbf{w} = \mathbf{u}$, also expecting quadratic convergence (cf. Sect. 3.3).

FIGURE 1 shows the convergence of **JD** for these choices when we restart at every iteration (taking $\mathbf{v}_0 = \mathbf{w}_0 = \mathbf{u}$) and FIGURE 2 shows the convergence for full **JD** with $\mathbf{W} = \mathbf{V}$. In these figures, $\log_{10}\|\mathbf{r}\|/c$ is plotted, where $\mathbf{r}$ is the residual of the Petrov-Ritz pair and c is the norm of the initial residual. As can be seen clearly from FIGURE 1, the speed of convergence confirms our expectations. Taking the proper projections has a dramatic influence on the speed of convergence, changing linear into quadratic behavior. Notice that there is hardly any difference in the speed of convergence for the last two cases.

By comparing FIGURE 1 with FIGURE 2 we can see the benefits of an increasing search and test space: it has an accelerating effect, changing linear into superlinear convergence and even the quadratic convergence is faster (the cases 2 and 3 coincide in the figure). In fact, there is not much difference between the three choices.

REMARK 9.1. From the point of view of overall performance and efficiency, we recommend the second choice. The additional matrix multiplication (compared with the first choice) with $\mathbf{B}$ can be compensated by combining its computation with the computation of the residual but this cannot be done for case 3 where the transposed matrix $\mathbf{B}^*$ is involved.

FIG. 1. *Restarted* **JD**

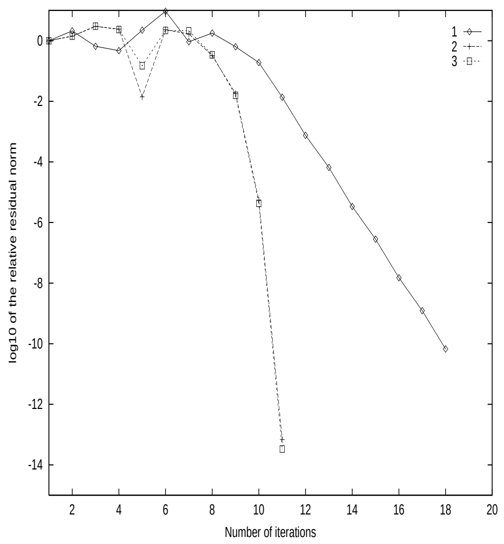
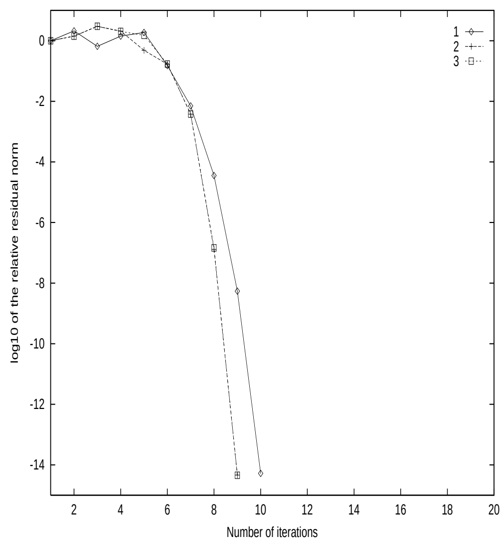


FIG. 2. *Full* **JD**



Quadratic versus cubic. In Section 3.2 the convergence with left eigenvectors is discussed. The statements made in that section about the speed of convergence are nicely confirmed by our numerical experiments, if we make the following choices for $\widetilde{\mathbf{w}}$, $\mathbf{w}$ and $\widetilde{\mathbf{u}}$:

1. $\widetilde{\mathbf{w}} = \widetilde{\mathbf{u}} = \mathbf{u}$, $\mathbf{w} = \mathbf{z}$, where $\mathbf{z}$ is the left Petrov-Ritz vector. This should lead to faster than linear convergence (cf. TH. 3.9);
2. $\widetilde{\mathbf{w}} = \widetilde{\mathbf{u}} = \mathbf{u}$, $\mathbf{w} = \mathbf{z}$, where $\mathbf{z}$ is the approximation for the left eigenvector obtained by solving the adjoint correction equation. This should lead to quadratic convergence (cf. REMARK 3.11);
3. $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}, \widetilde{\mathbf{u}} = \mathbf{B}^*\mathbf{z}, \mathbf{w} = \mathbf{z}$, where $\mathbf{z}$ is as above. Now we may expect cubic convergence, according to the last part of REMARK 3.11.

FIGURE 3 shows the convergence of **JD** for these choices when we restart at every iteration (with $\mathbf{v}_0 = \mathbf{u}$ and $\mathbf{w}_0 = \mathbf{z}$), and FIGURE 4 shows the convergence for full **JD** where now the test space is spanned by the approximations $\mathbf{z}$ of left eigenvector. Again, the speed of convergence is in line with our expectations. Using the left Petrov-Ritz vector (cf. Sect. 5.2) speeds up the convergence, which is now superlinear. Solving the adjoint correction equation and using the approximation to the left eigenvector results in quadratic, or even cubic speed of convergence (note the reduction of the relative residual norm from 10^{-5} to 10^{-15} in the final step), when the proper projections are used. And in addition, for the last two choices, one obtains the left eigenvector almost for free.

FIGURE 4 shows the accelerating effect of increasing search and test space.

FIG. 3. *Restarted* **JD** *using left Petrov-Ritz vectors*

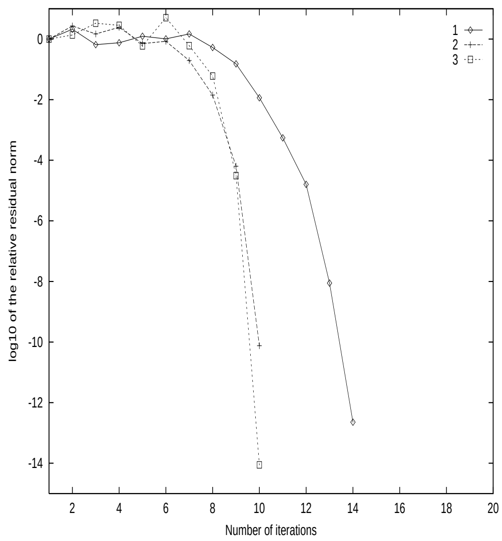
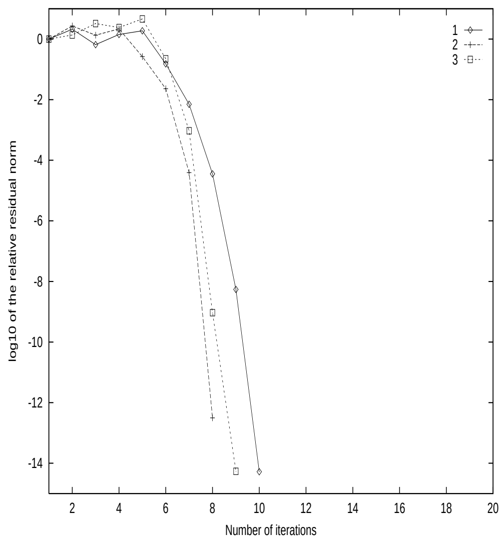


FIG. 4. *Full* **JD** *using left Petrov-Ritz vectors*



REMARK 9.2. Using the left Petrov-Ritz vector speeds up the convergence, but there is a catch: it may happen that this left Petrov-Ritz vector does not converge and this may result in slow or even no convergence for the **JD** process.

REMARK 9.3. Incorporating (approximations to) the left eigenvector in **JD** improves the speed of convergence, but at the cost of solving the adjoint correction equation (cf. (21)). This almost doubles the computational work, which is in general not compensated through a reduction in the number of iterations. Therefore, it appears that such a scheme can only be efficient when used for applications where both left and right eigenvectors are desired.

9.2. Reducing a generalized eigenproblem to a standard one. Now we consider an example of order 80. The nonsymmetric matrix $\mathbf{A}$ is tridiagonal and has the following non-zero entries (all other entries are zero):

$$a_{ij} = \begin{cases} i & \text{if } j = i, \\ 1 & \text{if } j = i+1, \\ -1 & \text{if } j = i-1, \end{cases}$$

and the symmetric matrix $\mathbf{B}$ is pentadiagonal, with the following non-zero entries:

$$b_{ij} = \begin{cases} 2 & \text{if } j = i, \\ -1 & \text{if } j = i+1, \\ -1 & \text{if } j = i-1, \\ 1 & \text{if } i = 1 \text{ and } j = n, \\ 1 & \text{if } i = n \text{ and } j = 1. \end{cases}$$

Note that $\mathbf{B}$ is positive-definite. This allows for the construction of a $\mathbf{B}$-orthonormal basis, i.e., $\mathbf{V}^*\mathbf{B}\mathbf{V} = I$. We selected $\mathbf{W} = \mathbf{V}$, and then the projected generalized eigenproblem reduces to a standard one. If $\mathbf{z}$ is the approximate solution of the correction equation, the set $[\,\mathbf{V}_k, \mathbf{z}\,]$ is $\mathbf{B}$-orthonormalized with results in $\mathbf{V}_{k+1}$, via the modified Gram-Schmidt (*ModGS$_B$*) procedure (see e.g. [12, 23]):

```
for i = 1, ..., k do:
    α := v_i^* B z;
    z := z − α v_i;
end;
β := ||z||_B;
v_{k+1} := z/β.
```

Here we introduced the $\mathbf{B}$-norm of a vector: $||\mathbf{z}||_B = (\mathbf{z}^*\mathbf{B}\mathbf{z})^{\frac{1}{2}}$. For an efficient implementation of this $\mathbf{B}$-orthogonalization process it is convenient to store the matrix $\mathbf{BV}$ in addition to the matrix $\mathbf{AV}$, which is necessary for the computation of the projected matrix $\mathbf{V}^*\mathbf{A}\mathbf{V}$.

The in absolute value largest eigenvalue of this matrix pair is real and its value is

$$\lambda = 34865.927904249\ldots$$

This eigenvalue is well separated from the other eigenvalues. We have tried to obtain an approximation for this eigenvalue with our **JD** method (Alg. 2). The starting vector $\mathbf{v}_1$ is chosen as $\alpha(1,\ldots,1)^T$, with α such that the $\mathbf{B}$-norm of $\mathbf{v}_1$ equals 1. The correction equation is solved approximately with m steps of GMRES with initial guess 0 and without preconditioning.

According to (22), the correction equation is embedded in the entire n-space with $\mathbf{w} = \mathbf{u}$ and $\widetilde{\mathbf{w}} = \widetilde{\mathbf{u}} = \mathbf{B}\mathbf{u}$ (recall that $\mathbf{B}$ is symmetric). The algorithm is restarted every 10 iterations with the current eigenvector approximation, i.e., when $k = \dim(\mathrm{span}(\mathbf{V})) = 10$ in Algorithm 2 we set $k = \ell = 1$ and $\mathbf{v}_1 = \mathbf{u}$. The eigenvector approximations $\mathbf{u}$ were normalized to have $\mathbf{B}$-norm 1 and the algorithm was stopped if the residual norm is smaller than 10^{-8}.

In Table 1 we have listed the number of outer iterations for convergence for different numbers of GMRES steps: from 5 up to 30. We compare the results of this **JD** variant with the variant for which $\widetilde{\mathbf{w}} = \mathbf{B}\mathbf{u}$, $\mathbf{w} = \mathbf{B}^{-*}\mathbf{u}$, $\widetilde{\mathbf{u}} = \mathbf{u}$. The latter approach corresponds to **JD** with $\widetilde{\mathbf{u}} = \mathbf{w} = \widetilde{\mathbf{w}} = \mathbf{u}$ applied to the standard eigenproblem $\mathbf{B}^{-1}\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x}$ (cf. Remark 3.6), and has been discussed in detail in [3]. Note that the second variant requires inversion of $\mathbf{B}^*$ (or exact solution of a system involving $\mathbf{B}^*$). In order to have a fair comparison we terminate this process as soon as the eigenvalue approximation has reached the same accuracy as obtained with the first, inversion-free, variant. From Table 1 we see that convergence is much faster for the first approach. Moreover, the work per iteration for the second variant is 50% more. This is reflected in the total number of matrix-vector multiplications (MVs), also given in the table, when we take the numbers of GMRES iterations into account.

Table 1

Example Sect. 9.2. Number of outer iterations for different inner iteration processes.

GMRES	**JD** Ref. [3]		**JD** Alg. 2	
m	# iter	# MVs	# iter	# MVs
5	3490	62805	91	1082
10	151	4953	29	618
15	46	2163	20	610
20	29	1767	17	674
25	20	1485	12	574
30	20	1770	11	622

Table 2

Example Sect. 9.2. Convergence history of the inversion-free **JD** *method with 30* GMRES *steps.*

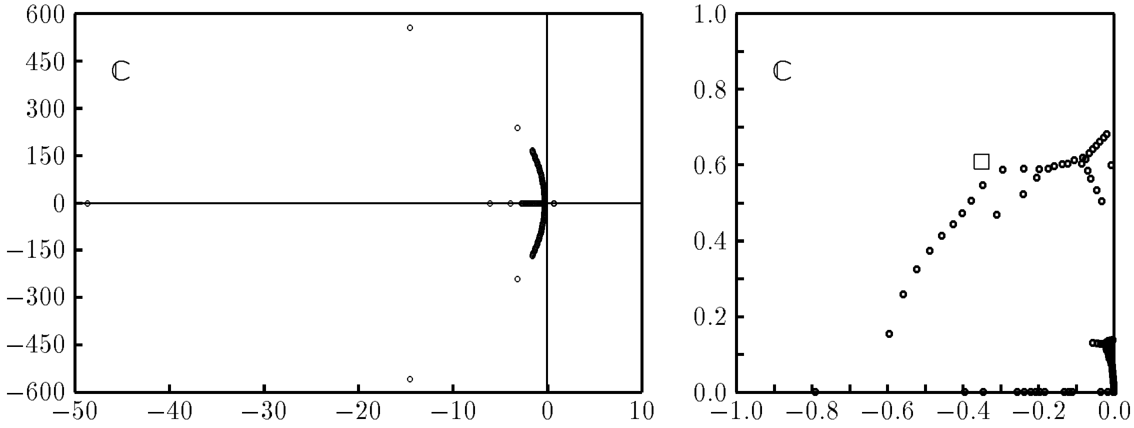
iteration	eigenvalue approximation	residual norm	residual norm GMRES
1	810.000000000	1135.79	2.469E−2
2	13206.799065923	4053.61	2.728E−1
3	13274.221312254	3812.23	2.913E−1
4	32278.051603129	1897.00	1.005E−1
5	33629.919920062	636.30	2.331E−1
6	34809.830442647	489.94	2.791E−2
7	34865.920209700	12.12	2.473E−3
8	34865.927902280	2.676E−2	2.227E−2
9	34865.927904258	1.113E−3	3.824E−3
10	34865.927904250	2.503E−6	3.199E−3
11	34865.927904249	8.265E−9	

When we increase the number of GMRES steps, then the convergence is improved for this example. This is not necessarily the case, as will be shown by the example in Section 9.3. For 30 GMRES steps convergence is reached in only 11 outer iterations. The convergence history for this inversion-free process is presented in Table 2. In the second column we have listed the eigenvalue approximations. Note that the true eigenvalue is reproduced up to machine precision in the final iteration. In the third column the residual norm of the eigenpair is shown. We observe that the convergence is at least more than linear, although the correction equations are solved with a very modest accuracy, as can be seen from the last column.

9.3. How to include a preconditioner?. Our next example is from a magnetohydrodynamics (MHD) model, where the interaction of hot plasmas and a magnetic field is studied. These MHD phenomena occur, e.g., in the solar corona and in thermonuclear fusion reactors. The dynamical behavior of magnetically confined plasmas is described by the MHD equations, which form a system of coupled nonlinear PDEs. The stability analysis of the linearized MHD equations leads to a generalized non-Hermitian eigenproblem. For more details on the physical background, see for instance [11].

The matrix $\mathbf{A}$ in this MHD-eigenvalue problem is non-Hermitian and the matrix $\mathbf{B}$ is positive-definite Hermitian. Both matrices are block tridiagonal with rather

FIG. 5. *The spectrum of the MHD test problem.*
The left figure gives an overview of the complete spectrum, while the right figure shows an amplification of the relevant part. Note that the figures have different scalings. Correct eigenvalues are shown (○) and the location of the target (□).



dense blocks. Quite large MHD eigenproblems have been successfully solved with a generalized nonsymmetric Lanczos procedure [5] and with an implicitly restarted Arnoldi method [15]. The latter method was a modification of a method proposed by Sorensen [30]. In both methods a Shift-and-Invert strategy is used, which requires the LU factorization of the shifted matrix $\mathbf{A} - \mu\,\mathbf{B}$. The additional storage requirements due to the L and U factors put severe limitations on the maximum problem size that can be handled with these methods on a given computer. In the Jacobi-Davidson algorithm the factorization of either matrix is avoided, which may in principle enable plasma physicists to study larger matrix problems. Several other algorithms that avoid factorization of a matrix have been presented in the literature, see e.g. [26, 27], but to our knowledge they only apply well to the symmetric positive definite case, i.e. $\mathbf{A}$, $\mathbf{B}$ symmetric and $\mathbf{B}$ positive definite.
What makes this problem extremely difficult is that the eigenvalues of interest are in the interior of the spectrum, see FIGURE 5. In fact, there are may large eigenvalues, and almost any approach that avoids inversion, like for instance the standard Arnoldi method, tends to find these large dominating eigenvalues. In this section we will study a very small MHD test problem, in order to see whether an inverse free Jacobi-Davidson iteration method is feasible at all, and also in order to get an impression how well the Jacobi-Davidson correction equation has to be solved.

The MHD test problem, that we will solve with the Jacobi-Davidson method, is obtained from [15]. The order of the matrices is $n = 416$, the size of the blocks is 16 by 16. The interesting part of the spectrum in MHD problems is determined by an interior branch of eigenvalues, known as the Alfvén spectrum. The relevant part of the spectrum, which includes the Alfvén branch is shown in the right figure of FIGURE 5. Note the strong clustering of unwanted eigenvalues around the origin; other much larger eigenvalues (the sound waves) are shown in left figure of FIGURE 5.

In order to force convergence towards interior eigenvalues, we select the Petrov-Ritz values θ that are closest to some target value τ, i.e. we search for the eigenvalue closest to τ. For τ we take $\tau = -0.3 + 0.65\,\mathrm{i}$, indicated by the square box (□) in FIGURE 5. As in Section 9.2 we construct a $\mathbf{B}$-orthonormal basis, starting with

$\mathbf{v}_1 = \alpha(1, \ldots, 1)^T$, with α such that the $\|\mathbf{v}_1\|_B = 1$.
We compare the results for two different forms for the correction equation:

(a) the embedded correction equation (22)

(b) and the augmented correction equation (23),

and we take $\mathbf{w} = \mathbf{u}$ and $\widetilde{\mathbf{w}} = \widetilde{\mathbf{u}} = \mathbf{B}\mathbf{u}$ for both situations.

It turns out that without preconditioning the correction equation was not solved sufficiently accurate to achieve convergence to the desired eigenvalue.

For the augmented correction equation we follow the prescription of (37) and (38), where we explicitly compute $\mathbf{y}$ and ν. For $\mathbf{K}$ we take the block diagonal part of $\mathbf{A} - \tau\,\mathbf{B}$, with the blocks 2×2 block matrices (i.e., the blocks in $\mathbf{K}$ have size 32×32). Note that $\mathbf{K}$ is computed only once, we do not update the preconditioner if the eigenvalue approximation is closer to λ than τ.

We precondition the embedded correction equation with $\mathbf{K}$ without any modification. We use the same $\mathbf{K}$ as for the augmented correction equation. In contrast to the augmented correction equation (23), the embedded equation (22) is formulated in the whole space and it is an option to apply $\mathbf{K}$ without any modification. However, we will show that this is not an advisable option. In exact arithmetic, the augmented formulation is equivalent to the projected one. This seems to be the case also in finite precision arithmetic. Therefore, if the formulation using projections is preferred, we advise to project the preconditoner as well.

The correction equations are solved approximately with m steps of full GMRES with initial guess 0. The maximum dimension of the subspaces $\mathcal{W}_k$ and $\mathcal{V}_k$, that are constructed in the iteration process, is 50 and we restart with the current eigenvector approximation. Eigenvector approximations are normalized to have $\mathbf{B}$-norm 1 and the algorithm is terminated when the residual norm of the approximate eigenpair is smaller than 10^{-8}.

In TABLE 3 we present the total number of outer iterations necessary to achieve convergence to the desired eigenvalue. We do this for the two different inner iteration processes, where we either solve the embedded correction equation or the augmented correction equation, each approximately with m steps of GMRES. We vary the number of GMRES steps m from 15 up to 120.

From TABLE 3 we observe that convergence is already achieved when we approximate the solution of the augmented correction equation with only 15 GMRES steps. Convergence is in general obtained in fewer iterations for the augmented correction equation with an augmented preconditioner than for the embedded correction equation with unmodified preconditioner (except for large m ($m \geq 80$): then the results are comparable).

Note that simply increasing the number of GMRES steps m, that is selecting a better preconditioner, will not a priori lead to better convergence results. For instance, for $m = 45$ we need 29 outer iterations for convergence with the augmented correction equation, whereas for $m = 50$ the number of outer iterations is 42. An explanation for this is suggested by the path that the approximate eigenvalues follow to the desired eigenvalue. It turns out that for $m = 50$ the convergence is much more affected by nearby other eigenvalues than for $m = 45$.

In FIGURE 6 we have plotted the $\log_{10}$ of the residual norm of the eigenpair approximation as a function of the outer iteration number. The augmented correction equation is solved approximately with 120 GMRES steps ($\star$), 80 GMRES steps ($\circ$) and 40 GMRES steps ($\bullet$). The residual norm of the approximate solution of the

TABLE 3
Example Sect. 9.3. Number of outer iterations for different inner iteration processes.

GMRES	Embedded Correction Equation	Augmented Correction Equation
m	# J-D iterations	# J-D iterations
15	no conv	197
20	133	48
25	84	77
30	75	40
35	47	34
40	41	33
45	41	29
50	34	42
55	31	27
60	35	29
65	29	27
70	26	22
75	37	25
80	24	24
85	24	24
90	29	25
95	36	19
100	21	20
105	17	18
110	16	17
115	13	21
120	11	16

augmented correction equation is displayed in FIGURE 7.

In FIGURE 6 we observe that the convergence is asymptotically quadratic if the correction equation is solved with high accuracy (120 GMRES steps). This mimics the situation where we do exact inverse. If we decrease the level of accuracy for the solution of the correction equation, that is if we use only 80 or 40 GMRES steps, then the convergence has a more linear behavior. An explanation may be deducted from FIGURE 7, where we see that with 120 steps of GMRES the linear systems are solved very accurately during the final iterations, whereas for 80 or 40 steps only a modest accuracy is achieved for the approximate solution of the correction equation, even during the final iterations. The results for 120 GMRES steps in FIGURE 7 indicate that the condition number of the correction equation improves during the convergence process, as might have been anticipated, since the eigenpair approximation moves towards the eigenpair. FIGURES 6 and 7 also illustrate that the progress made during the initial iterations is virtually the same, whether we solve the correction equation rather inaccurately (with 40) or to high accuracy (120 GMRES steps); this indicates an relatively early stagnation in the GMRES inner iteration process. Therefore it is probably more economical to solve the correction equation during the initial outer iterations with only a limited number of inner iteration steps and to increase this number as the convergence proceeds; see also Section 9.4

FIG. 6. *Convergence history MHD problem ($n = 416$): norm of the residual vector* $\mathbf{r}$. *The augmented correction equation is solved approximately with 120* GMRES *iteration steps* ($\star$), *80* GMRES *iteration steps* ($\circ$) *and 40* GMRES *iteration steps* ($\bullet$).

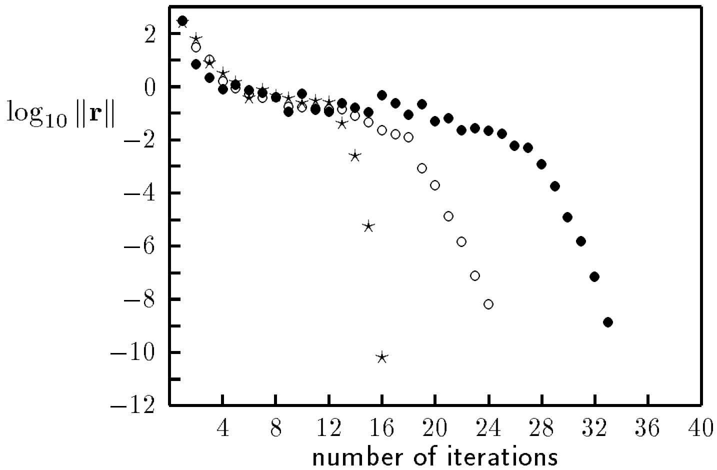
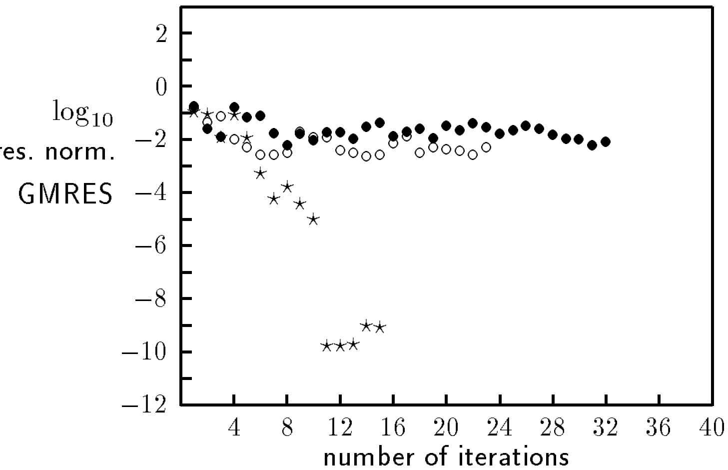


FIG. 7. *Residual norm for the approximate solution of the augmented correction equation obtained with m steps of the* GMRES *algorithm: $m = 120$ ($\star$), $m = 80$ ($\circ$) and $m = 40$ ($\bullet$).*



In this example we have seen that it is in principle possible to use the Jacobi-Davidson method for interior eigenvalues without the necessity for exact inversion of any matrix. The total number of matrix evaluations for this small example makes an iterative method completely unattractive with respect to a direct method. However, if we are in the situation that we can not invert any of the involved matrices, and if the distribution of the eigenvalues for the given problem is more or less the same as for our small test problem, then we see that is is not necessary to solve the correction equation very accurately. For the test problem the 11 Jacobi-Davidson steps with the accurate solver (120 steps with GMRES) results in 3632 matrix vector operations, whereas the 75 Jacobi-Davidson steps with the more inaccurate solver (20 steps of GMRES) requires 'only' 1976 iteration steps. Unfortunately, it is impossible to predict the proper choice for the number of GMRES steps.

This example really tells us that in practice we will need rather powerful preconditioners for the correction equation.

9.4. The computational costs. In view of our theoretical results in Section 3.1, we expect a faster converging **JD** process if the correction equation is solved more accurately. The numerical results in the previous subsections are in line with these observations: the number of outer iterations tends to decrease if the number of inner iterations increases. Unfortunately, a more accurate solution of the correction equation will involve more computational costs. The example in this section will illustrate that these costs can be compensated for by the faster convergence of the outer iteration.

For problems of interest, the matrices will be sparse, and a few iteration steps may not be expected to yield an accurate eigenpair approximation. Therefore, the vector updates and inner products, both in the outer iteration as well as in the inner iteration, will form a substantial part of total computational effort: to get an impression of the total amount of work to compute an eigenpair it is not enough to count the number of MVs.

Our example from the previous subsection does not give a realistic impression of the trade-offs in the computational costs: this model example is very small and a feasable preconditioner for large realistic MHD examples is still not available.

As in Section 9.1 we take a Dielectric Waveguide problem from the "Test Matrix Collection" [2]. Except for the order, which is now 782, the present problem has the same characteristics as the smaller one in Section 9.1. Again we search for the eigenvalue λ with largest real part ($\lambda \approx 2523$) by selecting the Petrov-Ritz value with largest real part. We precondition with the ILU(0) of $\mathbf{A} - \tau\mathbf{B}$, with $\tau = 2500$.

The eigenvalue with largest real part is almost double, which makes this example more difficult than the one in Section 9.1. The 5 rightmost eigenvalues (computed with **JD**) are (in 5 decimal places):

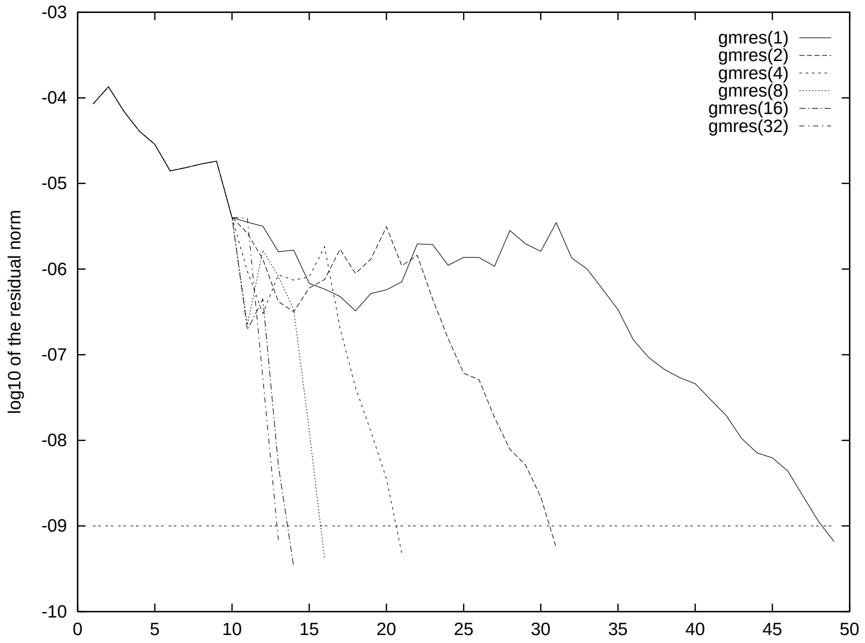
$$
\begin{aligned}
\lambda_1 &= 2.5233e03 - i\,3.1674e{-}05,\\
\lambda_2 &= 2.4843e03 + i\,1.0288e{-}04,\\
\lambda_3 &= 1.2640e03 - i\,2.1413e{-}04,\\
\lambda_4 &= 5.6467e02 - i\,1.3443e{-}05,\\
\lambda_5 &= -1.1373e03 - i\,2.7123e{-}04.
\end{aligned}
$$

We select $\mathbf{w} = \widetilde{\mathbf{w}} = \mathbf{Bu}$ and $\widetilde{\mathbf{u}} = \mathbf{u}$. Observe that the preconditioner has to map the image space in the correction equation to the domain space (cf. Sect. 3.3 and 7.1). We incorporate the preconditioner as explained in Theorem 7.4. Our test space is spanned by $\mathbf{BV}$.

As an initial guess for $\mathbf{v}$ and $\mathbf{w}$ we take the normalized vector with all coordinates equal. In all runs, in the first 10 **JD** sweeps, we solve the correction equation with 1 step of preconditioned GMRES; in the subsequential sweeps we allow more GMRES steps. Such an approach was already suggested at the end of Section 9.3. This may be motivated by the fact that that we find the exact eigenvector in the next step if we solve the correction equation exactly with λ instead of θ: actually we replaced λ by θ arguing that θ is the best approximation of λ that is available (cf. Sect. 2). However, especially in the initial stage of the process, θ may be worse than, say, τ. Since the present preconditioner is designed for a correction equation with τ rather θ, the result of 1 step of preconditioned GMRES applied to the "θ-correction equation" will actually approximate the solution of the "τ-correction equation" better, whereas the result of more steps of GMRES is a better approximation for the solution of the "θ-correction equation".

The results are shown in the FIGURES 8-10, where, for several values of m, the correction equation is solved with (at most) m steps of GMRES. FIGURE 8 gives the number of **JD** sweeps required to obtain an eigenpair approximation with a residual norm less than 10^{-9}. As may be expected this number decreases if m increases. For the number of MVs, shown in FIGURE 9, we have the opposite situation. In terms of computational work, there is not such a monotonic dependence on m. In FIGURE 10 we give the number of floating point operations (in millions) (neglecting the operations at low dimensional levels). The method turns out to be four times faster with $m = 8$ than with $m = 1$.

FIG. 8. *Number of* **JD** *iterations*



Arnoldi did not convergence within 80×10^6 flops.
In other examples, we did not obtain convergence with a few steps of GMRES, while in other examples 1 step of GMRES turned out to be the most efficient approach. What the best strategy is depends on the problem and, of course, on the quality of the preconditioner.

9.5. Computing several eigenvalues simultaneously. So far we have restricted our numerical tests to the computation of a single eigenvalue. In order to obtain several eigenvalues at the same time, we try a block variant of the basic Jacobi-Davidson algorithm (ALG. 2), that is similar to a block variant suggested for the classical Davidson method applied to standard eigenproblems [25].

For simplicity assume that the matrix $\mathbf{B}$ is Hermitian positive definite. We construct a $\mathbf{B}$-orthonormal basis with the modified Gram-Schmidt $\mathbf{B}$-orthogonalization process (*ModGS$_B$*), and solve the augmented correction equations (approximately) with $\mathbf{w} = \mathbf{u}$ and $\widetilde{\mathbf{w}} = \widetilde{\mathbf{u}} = \mathbf{B}\mathbf{u}$. The block variant has the form as in ALGORITHM 3. Note that we try to obtain approximations for ℓ eigenvalues simultaneously. At every outer iteration we increase the dimension of the subspace $\mathcal{V}_k$ by ℓ. The maximum dimension of the subspace is m. The restart is carried out with the ℓ current eigenvector approximations.

Fig. 9. *Number of MVs*

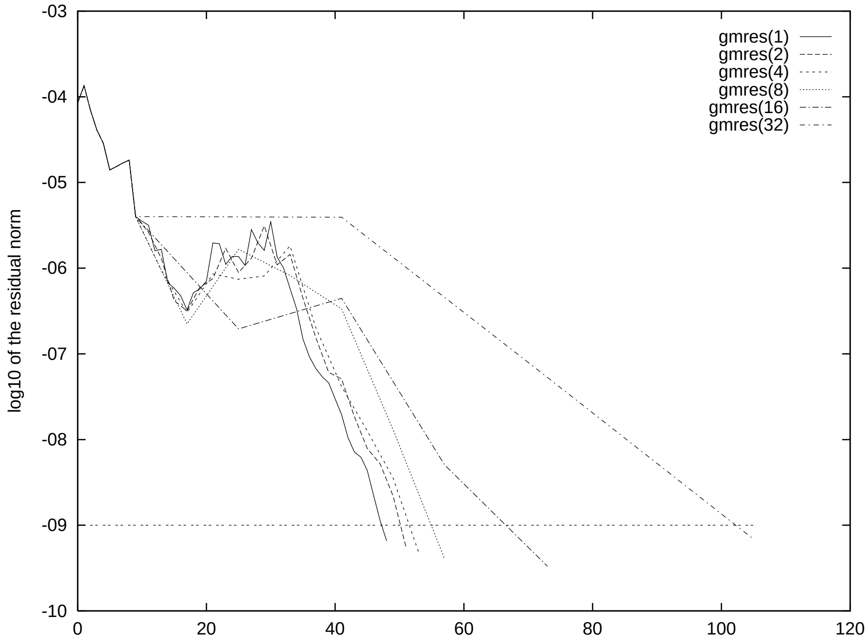
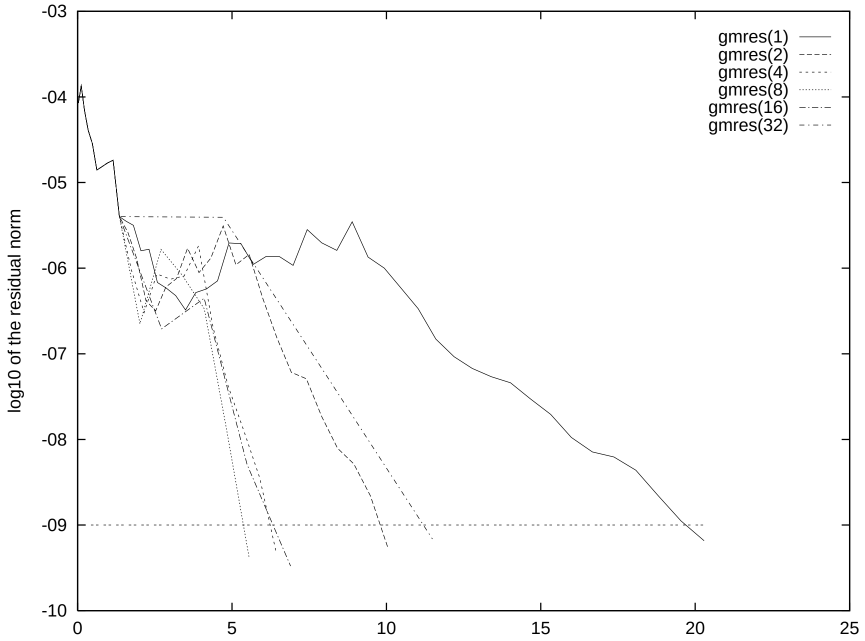


Fig. 10. *Number of flops* ($\times 10^6$)



As an alternative block variant, one can also combine Algorithm 2 with the block variant discussed here, i.e., at a certain stage in Algorithm 2 one restarts and switches over to the block variant described above. Another possibility for computing several eigenvalues is to incorporate deflation techniques, see for instance [23, 29, 8, 22].

We have applied this block variant for the MHD test problem (Sect. 9.3) and we have tried to reproduce the Alfvén spectrum. Therefore we have run the algorithm, for several suitably chosen targets, with $m = 48$ and we have computed approximations

ALGORITHM 3. *A block variant of Jacobi-Davidson*

Choose an initial $\mathbf{B}$-orthonormal matrix $\mathbf{V}_1 := [\mathbf{v}_1, \ldots, \mathbf{v}_\ell]$;
`For` $k = 1, 2, \ldots$ `do:`
(a) $\mathbf{W}_k^A := \mathbf{A}\mathbf{V}_k,\ \mathbf{W}_k^B := \mathbf{B}\mathbf{V}_k,\ H_k := \mathbf{V}_k^*\mathbf{W}_k^A$;
(b) Compute the ℓ desired eigenpairs $(\theta_{k,i}, y_{k,i})_{1\le i\le \ell}$ of H_k;
`For` $i = 1, \ldots, \ell$ compute:
$\mathbf{u}_{k,i} := \mathbf{V}_k y_{k,i},\ \mathbf{p}_{k,i} := \mathbf{W}_k^A y_{k,i},\ \mathbf{q}_{k,i} := \mathbf{W}_k^B y_{k,i}$,
$\mathbf{r}_{k,i} := \mathbf{p}_{k,i} - \theta_{k,i}\mathbf{q}_{k,i}$;
(c) `If` convergence `then` exit;
(d) For $i = 1, \ldots, \ell$
solve the augmented correction equation (approximately):

$$\begin{bmatrix} \mathbf{A} - \theta_{k,i}\mathbf{B} & \mathbf{q}_{k,i} \\ \mathbf{q}_{k,i}^* & 0 \end{bmatrix} \begin{bmatrix} \mathbf{z}_{k,i} \\ \varepsilon_{k,i} \end{bmatrix} = \begin{bmatrix} -\mathbf{r}_{k,i} \\ 0 \end{bmatrix};$$

(e) `If` $\dim(\mathbf{V}_k) \le m - \ell$
`then` $\mathbf{V}_{k+1} := \mathit{ModGS_B}(\mathbf{V}_k, \mathbf{z}_{k,1}, \ldots, \mathbf{z}_{k,\ell})$;
`else` $\mathbf{V}_{k+1} := \mathit{ModGS_B}(\mathbf{u}_{k,1}, \ldots, \mathbf{u}_{k,\ell}, \mathbf{z}_{k,1}, \ldots, \mathbf{z}_{k,\ell})$;
`end if`;
`end for`

for the $\ell = 4$ eigenvalues nearest to the target. For the initial matrix we have chosen: $\mathbf{V}_1 = \mathit{ModGS_B}(e_{201}, \ldots, e_{204})$, with e_j the j-th canonical unit vector. The eigenvector approximations $\mathbf{u}_{k,i}$ are normalized to have $\mathbf{B}$-norm unity. The algorithm is stopped when the residual norm of the eigenpair approximation nearest to the target is smaller than 10^{-10}.

We have solved the augmented correction equation with (at most) 100 steps of GMRES, using the same block Jacobi (left) preconditioning as in Section 9.3.

The results are given in TABLE 4. We have listed the target (τ), the number of outer iterations (# iter), the number of converged eigenvalues (# EVs), the minimum of the residual norms of the converged eigenpairs (min. res.), and the maximum of the residual norms of the converged eigenpairs (max. res.). We have used as criterion that an eigenpair approximation is considered to be converged when the residual norm is smaller than 10^{-6}. For eigenvalues close to the 'bifurcation' point (see FIG. 5; targets 5 to 11) the results are obtained with $\ell = 3$, $m = 45$ and stopping tolerance 10^{-7}, starting with $\mathbf{V}_1 = \mathit{ModGS_B}(e_{201}, \ldots, e_{203})$. The motivation for this is that in that region the eigenvalues are very close and consequently the eigenpairs are difficult to distinguish. This has also been experienced in ref. [15] for the generalized Lanczos method as well as for the shift-and-invert Arnoldi method. From TABLE 4 we see that 11 targets have been necessary to reproduce the entire Alfvén spectrum (34 eigenvalues for this test problem).

Acknowledgement.
We gratefully acknowledge stimulating discussions with Martin van Gijzen.

TABLE 4
Example Sect. 9.5. Results of the block variant applied to the MHD test problem.

target	# iter	# EVs	min. res.	max. res.
τ_1 = -0.6 + 0.25 i	16	3	6.06E−13	1.62E−08
τ_2 = -0.5 + 0.45 i	27	4	5.35E−13	2.51E−07
τ_3 = -0.325 + 0.525 i	22	4	9.94E−11	8.83E−10
τ_4 = -0.25 + 0.55 i	18	3	5.03E−12	3.33E−09
τ_5 = -0.2 + 0.65 i	26	3	1.42E−08	3.06E−07
τ_6 = -0.125 + 0.625 i	23	3	6.05E−08	8.07E−07
τ_7 = -0.075 + 0.625 i	26	3	5.03E−08	5.06E−07
τ_8 = -0.075 + 0.59 i	28	2	4.10E−08	1.50E−07
τ_9 = 0.0 + 0.525 i	24	3	1.62E−08	7.56E−08
τ_{10} = -0.04 + 0.68 i	27	3	2.35E−10	1.45E−08
τ_{11} = -0.0275+ 0.6225 i	25	3	2.58E−08	4.48E−07

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A. Newton. As **JD**, Newton improves approximate eigenvectors by corrections equations. This process produces sequences that converge asymptotically with asymptotic quadratic speed.

Newton corrects approximations of zeros of differentiable functions. In Section 7.2, we considered one approach where we tried to keep one component of the approximating eigenvector fixed (we kept the $\mathbf{u}$-direction fixed). However, it might seem to be more natural the keep the length of the approximating eigenvector fixed. Before commenting on the relation between **JD** and Newton, we formulate Newton for eigenvector approximation by normalized vectors.

We are interested in the normalized eigenvectors $\mathbf{x}$: $\|\mathbf{x}\| = 1$.
Let $\mathcal{S}_n$ be the n-sphere: $\mathcal{S}_n := \{\mathbf{y} \in \mathbb{C}^n \mid \|\mathbf{y}\| = 1\}$. Consider the map r from the n-dimensional space $\mathbb{C} \times \mathcal{S}_n$ into the n-dimensional space $\mathbb{C}^n$ given by

$$r(\vartheta, \mathbf{u}) := \mathbf{A}\mathbf{u} - \vartheta\,\mathbf{B}\mathbf{u} \quad \text{where} \quad \mathbf{u} \in \mathcal{S}_n \quad \text{and} \quad \vartheta \in \mathbb{C}. \tag{48}$$

The Newton process produces sequences $(\lambda_k, \mathbf{u}_k)$ such that

$$\lambda_{k+1} = \lambda_k + \varepsilon_k \quad \text{and} \quad \mathbf{u}_{k+1} = \frac{\mathbf{u}_k - \mathbf{f}_k}{\sqrt{1 + \|\mathbf{f}_k\|^2}} \quad \text{with} \quad \mathbf{f}_k \perp \mathbf{u}_k$$

where the corrections ε_k and $\mathbf{f}_k$ are the solutions of the residual equation involving the Jacobian Dr of r:

$$Dr_{|(\lambda_k, \mathbf{u}_k)}(\varepsilon_k, \mathbf{f}_k) = \mathbf{r}_k := r(\lambda_k, \mathbf{u}_k) = \mathbf{A}\mathbf{u}_k - \lambda_k \mathbf{B}\mathbf{u}_k$$

Since

$$Dr_{|(\vartheta, \mathbf{u})}(\varepsilon, \mathbf{f}) == -\varepsilon \mathbf{B}\mathbf{u} + (\mathbf{A} - \vartheta\,\mathbf{B})\mathbf{f}$$

the corrections satisfy

$$-\,\varepsilon_k \mathbf{B}\mathbf{u}_k + (\mathbf{A} - \lambda_k \mathbf{B})\mathbf{f}_k = \mathbf{r}_k. \tag{49}$$

Choose some vector $\mathbf{w}$ (e.g. $\mathbf{w} = \mathbf{u}_k$ or $\mathbf{w} = \mathbf{B}\mathbf{u}_k$). By multiplying (49) by $\mathbf{w}^*$, we see that

$$\varepsilon_k = \frac{\mathbf{w}^*(\mathbf{A} - \lambda_k \mathbf{B})\mathbf{f}_k - \mathbf{w}^* \mathbf{r}_k}{\mathbf{w}^* \mathbf{B}\mathbf{u}_k}.$$

Substituting this expression for ε_k in (49) leads to

$$\mathbf{f}_k \perp \mathbf{u}_k \quad \text{and} \quad \left(\mathbf{I} - \frac{\mathbf{B}\mathbf{u}_k\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{u}_k}\right)(\mathbf{A} - \lambda_k \mathbf{B})\mathbf{f}_k = \left(\mathbf{I} - \frac{\mathbf{B}\mathbf{u}_k\,\mathbf{w}^*}{\mathbf{w}^*\mathbf{B}\mathbf{u}_k}\right)\mathbf{r}_k. \tag{50}$$

The choice $\mathbf{w} = \mathbf{u}_k$ and λ_k such that $\mathbf{r} \perp \mathbf{u}_k$ simplifies the above relations a little.