A NEW JUSTIFICATION OF THE JACOBI–DAVIDSON METHOD FOR LARGE EIGENPROBLEMS

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Abstract. The Jacobi–Davidson method is known to converge at least quadratically if the correction equation is solved exactly, and it is common experience that the fast convergence is maintained if the correction equation is solved only approximately. In this note we derive the Jacobi–Davidson method in a way that explains this robust behavior.

Key words. Eigenvalue approximation, Jacobi–Davidson method, robustness,

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1. Introduction. In this paper we consider the large and sparse eigenvalue problem

$$Ax = \lambda x \tag{1.1}$$

or more generally the nonlinear eigenproblem

$$T(\lambda)x = 0 \tag{1.2}$$

where $A \in \mathbb{C}^{n\times n}$ and $T : D \to \mathbb{C}^{n\times n}$, $D \subset \mathbb{C}$ is a family of sparse matrices.

For the linear problem (1.1) iterative projection methods have proven to be very efficient if a small number of eigenvalues and eigenvectors are desired. Here the eigenproblem is projected to a subspace of small dimension which yields approximate eigenpairs. If an error tolerance is not met then the search space is expanded in an iterative way with the aim that some of the eigenvalues of the reduced matrix become good approximations of some of the wanted eigenvalues of the given large matrix.

Particularly efficient are Krylov subspace methods like the Lanczos and the Arnoldi algorithm which provide rapid convergence to well separated and extreme eigenvalues and corresponding eigenvectors. For interior eigenvalues these methods tend to exhibit difficulties which can be remedied by shift-and-invert techniques, i.e. by applying the method to the matrix $(A - \sigma I)^{-1}$ where σ denotes a shift which is close to the wanted eigenvalues.

However, for truly large eigenproblems it is very costly or even infeasible to solve the shift-and-invert equation $(A - \sigma I)x = y$ by a direct method as LU factorization, and an iterative method has to be employed to solve it approximately.

Unfortunately, methods like the Lanczos algorithm and the Arnoldi algorithm are very sensitive to inexact solutions of $(A - \sigma I)x = y$, and therefore the combination of these methods with iterative solvers of the shift-and-invert equation usually is inefficient (cf. [3, 5, 6, 11, 24, 25]).

An iterative projection method which is more robust to inexact expansions of search spaces than Krylov subspace methods is the Jacobi–Davidson method which was introduced approximately 10 years ago by Sleijpen and van der Vorst [27] for the linear eigenproblem (1.1), and which was extended to matrix pencils in [4], to polynomial eigenproblems in [26], and to the general nonlinear eigenvalue problem

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(1.2) in [2] and [31]. A survey has recently been given in [7], pseudo codes are contained in [1].

Usually the Jacobi–Davidson expansion of a search space $\mathcal{V}$ is derived as orthogonal correction t of a current Ritz pair (θ, x) which is the solution of the so called correction equation

$$(I - xx^H)(A - \theta I)(I - xx^H)t = -(A - \theta I)x, \quad t \perp x. \tag{1.3}$$

It has been shown in [27] that the expanded space $\text{span}\{\mathcal{V}, t\}$ contains the direction $(A - \theta I)^{-1}x$ which is obtained by one step of the Rayleigh quotient iteration. Hence, one can expect quadratic convergence if the correction equation is solved exactly, and the convergence is even cubic in the Hermitian case.

It is common experience that fast convergence is maintained if the correction equation (1.3) is solved only approximately. But the way the expansion of the search space was derived by Sleijpen and van der Vorst does not indicate why the Jacobi–Davidson method is more robust to inaccurate solutions of the correction equation than the expansion by the direction obtained by an inexact Rayleigh quotient iteration.

In this note we present an approach for deriving the correction equation (1.3) in a way that explains the robustness of the Jacobi–Davidson method with respect to inexact solves of (1.3). We do not discuss the behavior of the Jacobi–Davidson method if the correction equation is solved in a particular way like a Galerkin–Krylov subspace solver (cf. [25]), nor do we discuss the convergence properties of the inexact Rayleigh quotient iteration (cf. [10, 15, 16, 17, 18, 20, 28] or of the Jacobi–Davidson method if the correction equation is solved approximately up to a predetermined residual norm of (1.3) (cf. [20, 22, 28]) or a residual norm that is specified dynamically in the course of the algorithm (cf. [19, 21, 24, 29]). Assuming an arbitrary error of the true expansion we show that the correction equation (1.3) yields the most robust way to expand the search space such that the direction of the Rayleigh quotient iteration at the current approximation is contained in the new search space. Considering structured errors is beyond the scope of this note.

2. A geometric derivation of a robust search space expansion. Consider the linear eigenvalue problem (1.1). Let $\mathcal{V}$ be the current search space of an iterative projection method. Assume that $x \in \mathcal{V}$ with $\|x\| = 1$ is the current approximation to the eigenvector we are aiming at, and let $\theta = x^H Ax$ be the corresponding Rayleigh quotient. Because of its good approximation property we want to expand the search space by the direction of inverse iteration $v = (A - \theta I)^{-1}x/\|(A - \theta I)^{-1}x\|$.

However, in a truly large problem the vector v will not be accessible but only an inexact solution $\tilde{v} := v + e$ of $(A - \theta I)v = x$, and the next iterate will be a solution of the projection of (1.1) onto the space $\tilde{\mathcal{V}} := \text{span}\{\mathcal{V}, \tilde{v}\}$.

We assume that x is already a good approximation to an eigenvector of A. Then v will be an even better approximation, and therefore the eigenvector we are looking for will be very close to the plane $E := \text{span}\{x, v\}$. We therefore neglect the influence of the orthogonal complement of x in $\mathcal{V}$ on the next iterate and discuss the nearness of the planes E and $\tilde{E} := \text{span}\{x, \tilde{v}\}$. If the angle between these two planes is small, then the projection of (1.1) onto $\tilde{\mathcal{V}}$ should be similar to the one onto $\text{span}\{\mathcal{V}, v\}$, and the approximation properties of inverse iteration should be maintained. If this angle can become large, then it is not surprising that the convergence properties of inverse iteration are not reflected by the projection method.

We denote by $\phi_0 = \arccos(x^T v)$ the angle between x and v, and the relative error of $\tilde{v}$ by $\varepsilon := \|e\|$.

THEOREM 2.1. *The maximal possible acute angle between the planes E and $\tilde{E}$ is*

$$\beta(\varepsilon) = \begin{cases} \arccos\sqrt{1-\varepsilon^2/\sin^2\phi_0} & \text{if} \quad \varepsilon \le |\sin\phi_0| \\ \frac{\pi}{2} & \text{if} \quad \varepsilon \ge |\sin\phi_0| \end{cases} \tag{2.1}$$

Proof. For $\varepsilon > |\sin\phi_0|$ the vector x is contained in the ball with center v and radius ε, and therefore the maximum acute angle between E and $\tilde{E}$ is $\frac{\pi}{2}$.

For $\varepsilon \le |\sin\phi_0|$ we assume without loss of generality that $v = (1,0,0)^T$, $\tilde{v} = (1+e_1, e_2, e_3)^H$, and $x = (\cos\phi_0, \sin\phi_0, 0)^T$. Obviously the angle between E and $\tilde{E}$ is maximal, if the plane $\tilde{E}$ is tangential to the ball B with center v and radius ε. Then $\tilde{v}$ is the common point of ∂B and the plane $\tilde{E}$, i.e. the normal vector $\tilde{n}$ of $\tilde{E}$ has the same direction as the perturbation vector e:

$$e = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \end{pmatrix} = \gamma\tilde{n} = \gamma \begin{pmatrix} \cos\phi_0 \\ \sin\phi_0 \\ 0 \end{pmatrix} \times \begin{pmatrix} 1+e_1 \\ e_2 \\ e_3 \end{pmatrix} = \gamma \begin{pmatrix} e_3\sin\phi_0 \\ -e_3\cos\phi_0 \\ e_2\cos\phi_0 - (1+e_1)\sin\phi_0 \end{pmatrix}. \tag{2.2}$$

Hence, we have $e_1 = \gamma\sin\phi_0 e_3$, $e_2 = -\gamma\cos\phi_0 e_3$, and the third component yields

$$e_3 = \gamma(-\gamma\cos^2\phi_0 e_3 - (1+\gamma\sin\phi_0 e_3)\sin\phi_0) = -\gamma^2 e_3 - \gamma\sin\phi_0,$$

i.e.

$$e_3 = -\frac{\gamma}{1+\gamma^2}\sin\phi_0. \tag{2.3}$$

Moreover, from

$$\varepsilon^2 = e_1^2 + e_2^2 + e_3^2 = \gamma^2\sin^2\phi_0 e_3^2 + \gamma^2\cos^2\phi_0 e_3^2 + e_3^2 = (1+\gamma^2)e_3^2,$$

we obtain

$$\varepsilon^2 = \frac{\gamma^2}{1+\gamma^2}\sin^2\phi_0, \quad \text{i.e. } \gamma^2 = \frac{\varepsilon^2}{\sin^2\phi_0 - \varepsilon^2}.$$

Inserting into (2.3) yields

$$e_3^2 = \frac{1}{1+\gamma^2}\varepsilon^2 = \Big(1 - \frac{\varepsilon^2}{\sin^2\phi_0}\Big)\varepsilon^2,$$

and since the normal vector of E is $n = (0,0,1)^T$, we finally get

$$\cos\beta(\varepsilon) = \frac{e^T n}{\|n\| \cdot \|e\|} = \frac{e_3}{\varepsilon} = \sqrt{1 - \frac{\varepsilon^2}{\sin^2\phi_0}}.$$

□

Obviously for every $\alpha \in \mathbb{R}$, $\alpha \ne 0$ the plane E is also spanned by x and $x + \alpha v$. If $\tilde{E}(\alpha)$ is the plane which is spanned by x and a perturbed realization $x + \alpha v + e$ of $x + \alpha v$ then by the same arguments as in the proof of Theorem 2.1 the maximum angle between E and $\tilde{E}(\alpha)$ is

$$\gamma(\alpha,\varepsilon) = \begin{cases} \arccos\sqrt{1-\varepsilon^2/\sin^2\phi(\alpha)} & \text{if} \quad \varepsilon \le |\sin\phi(\alpha)| \\ \frac{\pi}{2} & \text{if} \quad \varepsilon \ge |\sin\phi(\alpha)| \end{cases} \tag{2.4}$$

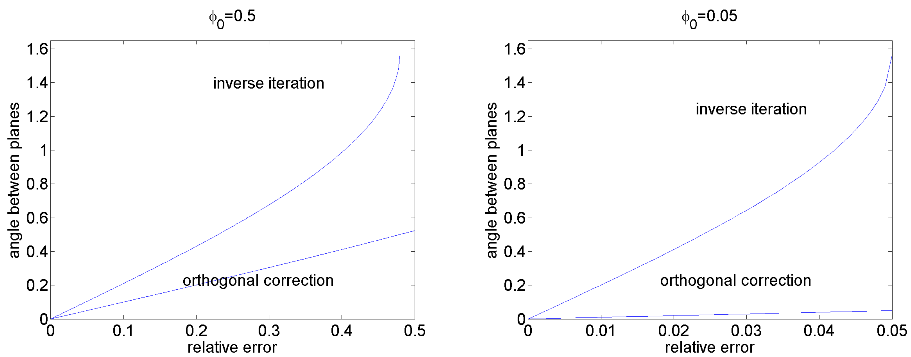

FIG. 2.1. *Maximum angle between exact and inexact planes*

where $\phi(\alpha)$ denotes the angle between x and $x + \alpha v$. Since the mapping

$$\phi \mapsto \arccos \sqrt{1 - \varepsilon^2 / \sin^2 \phi}$$

decreases monotonically the expansion of the search space by an inexact realization of $t := x + \alpha v$ is most robust with respect to small perturbations, if α is chosen such that x and $x + \alpha v$ are orthogonal, i.e. by

$$t = x - \frac{x^H x}{x^H (A - \theta I)^{-1} x} (A - \theta I)^{-1} x. \tag{2.5}$$

Then the maximum acute angle between E and $\tilde{E}(\alpha)$ satisfies

$$\gamma(\alpha, \varepsilon) = \begin{cases} \arccos \sqrt{1 - \varepsilon^2} & \text{if} \quad \varepsilon \leq 1 \\ \frac{\pi}{2} & \text{if} \quad \varepsilon \geq 1 \end{cases} . \tag{2.6}$$

Figure 2.1 shows the maximum angles between the planes $E = \text{span}\{x, v\}$ and $\tilde{E} = \text{span}\{x, \tilde{v}\}$ if $\tilde{v}$ is obtained by inexact evaluation of the direction of inverse iteration v and of the orthogonal correction t, respectively, for two angles $\phi_0 = 0.5$ and $\phi_0 = 0.05$ between x and v. It demonstrates that for a large angle ϕ_0 the robustness does not increase very much, but for small angles, i.e. in case where x is already quite accurate, the gain of robustness is essential.

3. Jacobi–Davidson method. Obviously, the expansion t in (2.5) of the current search space $\mathcal{V}$ is the solution of the equation

$$(I - xx^H)(A - \theta I)(I - xx^H)t = (A - \theta I)x, \quad t \perp x. \tag{3.1}$$

This is the so called correction equation of the Jacobi–Davidson method which was derived by Sleijpen and van der Vorst in [27] as a generalization of an approach of Jacobi [9] for improving the quality of an eigenpair of a symmetric matrix. Hence, the Jacobi–Davidson method is the most robust realization of an expansion of a search space such that the direction of inverse iteration is contained in the expanded space in the sense that it is least sensitive to inexact solves of linear systems $(A - \theta I)v = x$.

Similarly, we obtain the Jacobi–Davidson expansions for more general eigenvalue problems. Consider the generalized eigenvalue problem

$$Ax = \lambda Bx \tag{3.2}$$

where B is nonsingular. Then given an approximation (θ, x) to an eigenpair the inverse iteration is defined by $v := (A - \theta B)^{-1} Bx$. Again, we expand the current search space by $t := x + \alpha v$, where α is chosen such that x and $x + \alpha v$ are orthogonal, i.e. by

$$t = x - \frac{x^H x}{x^H (A - \theta B)^{-1} Bx} (A - \theta B)^{-1} Bx,$$

and this is the solution of the well known correction equation

$$\Big(I - \frac{Bxx^H}{x^H Bx}\Big)\Big(A - \theta B\Big)\Big(I - \frac{xx^H}{x^H x}\Big) t = (A - \theta B)x, \quad t \perp x \tag{3.3}$$

of the Jacobi–Davidson method introduced in [4].

If B is Hermitian and positive definite, and angles are measured with respect to the scalar product $\langle x, y \rangle_B := x^H By$, then the robustness requirement $\langle x, x + \alpha v \rangle_B = 0$ yields the expansion

$$t = x - \frac{x^H Bx}{x^H B (A - \theta B)^{-1} Bx} (A - \theta B)^{-1} Bx,$$

which is the solution of the symmetric correction equation (cf. [26])

$$\Big(I - \frac{Bxx^H}{x^H Bx}\Big)\Big(A - \theta B\Big)\Big(I - \frac{xx^H B}{x^H Bx}\Big) t = (A - \theta B)x, \quad t \perp_B x. \tag{3.4}$$

Finally, we consider the nonlinear eigenproblem (1.2) where the elements of T are assumed to be differentiable with respect to λ. Then given an eigenpair approximation (θ, x) the direction of inverse iteration is $v = T(\theta)^{-1} T'(\theta)x$. $t := x + \alpha v$ is orthogonal to x if

$$t = x - \frac{x^H x}{x^H T(\theta)^{-1} T'(\theta)x} T(\theta)^{-1} T'(\theta)x,$$

and this is the solution of the correction equation

$$\Big(I - \frac{T'(\theta)xx^H}{x^H T'(\theta)x}\Big) T(\theta) \Big(I - \frac{xx^H}{x^H x}\Big) t = T(\theta)x, \quad t \perp x. \tag{3.5}$$

which was discussed in [2, 31], and for polynomial eigenvalue problems in [26].

In a similar way one can motivate a two-sided Jacobi–Davidson method. For highly nonnormal matrices it is often advantageous to replace the Rayleigh quotient by Ostrowski's two-sided Rayleigh quotient [23]

$$\theta(u, v) = \frac{v^H Au}{v^H u} \tag{3.6}$$

where v and u denotes an approximate left and right eigenvector of A, respectively, and to improve these approximations by solving simultaneously the two linear systems

$$(A - \theta I)\tilde{u} = u \quad \text{and} \quad (A^H - \overline{\theta} I)\tilde{v} = v. \tag{3.7}$$

More generally, new approximations to v and u can be extracted from left and right subspaces which are expanded such that the solutions of equation (3.7) at the current approximation (θ, u, v) are contained in the augmented spaces. For robustness reasons we expand the spaces by

$$s = u + \alpha(A - \theta I)^{-1}u \quad \text{and} \quad t = v + \beta(A^H - \overline{\theta} I)^{-1}v,$$

and we choose α and β such that $s \perp u$ and $t \perp v$, i.e.

$$\alpha = -\frac{\|u\|^2}{u^H(A - \theta I)^{-1}u} \quad \text{and} \quad \beta = -\frac{\|v\|^2}{v^H(A^H - \overline{\theta} I)^{-1}v}.$$

Hence, s is a solution of the projecetd problem

$$\Big(I - \frac{up^H}{p^H u}\Big)(A - \theta I)(I - uu^H)s = (A - \theta I)u, \quad s \perp u,$$

for some $p \in \mathbb{C}^n$, and for consistency reasons we choose $p = v$, since by construction $(A - \theta I)u \in v^{\perp}$. Similarly the correction equation for t reads

$$\Big(I - \frac{vu^H}{u^H v}\Big)(A^H - \overline{\theta} I)(I - vv^H)t = (A^H - \overline{\theta} I)v, \quad t \perp v,$$

These corresction equations for the two-sided Jacobi–Davidson method were derived by Hochstenbach and Sleijpen [8]. Additionally, they proposed a different way of expanding the search subspaces requiring the bi-orthogonality of the constructed bases.

It is obvious how this two-sided approach can be adapted to generalized and nonlinear eigenvalue problems.

4. Inexact Krylov subspace methods. In [13] Meerbergen and Rose investigate an inexact shift-and-invert Arnoldi method for the generalized eigenvalue problem $Ax = \lambda Bx$. They demonstrate the superior numerical performance of a Cayley transformation over that of a shift–invert transformation within an Arnoldi method when using an iterative linear solver. Similarly Lehoucq and Meerbergen [11] showed that the Cayley transformation leads to a more robust eigensolver than the usual shift-and-invert transformation when the linear systems are solved inexactly within the rational Krylov method.

Aiming at the eigenvalue $\tilde{\lambda}$ that is closest to some shift σ in both methods the current search space $\mathcal{V}$ is expanded by

$$t_{SI} = (A - \sigma B)^{-1}Bx \tag{4.1}$$

where x is a Ritz vector with respect to $\mathcal{V}$ corresponding to the Ritz value θ closest to σ.

Since

$$(A - \sigma B)^{-1}(A - \theta B)x = x + (\sigma - \theta)(A - \sigma B)^{-1}Bx$$

and $x \in \mathcal{V}$, this expansion is equivalent to the one given by the Cayley transformation

$$t_C = (A - \sigma B)^{-1}(A - \theta B)x \tag{4.2}$$

if (4.1) and (4.2) are evaluated in exact arithmetic.

However, since $|x^H t_{SI}|/\|t_{SI}\| \to 1$ as $\theta \to \tilde{\lambda}$ and x approaches an eigenvector corresponding to $\tilde{\lambda}$ whereas $x^H t_C/\|t_C\| \to 0$, the considerations in Section 2 indicate that we may expect a more robust behavior of Arnoldi's method and the rational

Krylov method, if the search space is expanded by an inexact realization of t_C than by an approximation to t_{SI}.

Similar considerations hold for the nonlinear Arnoldi method [12, 30] for problem (1.2). There the expansion of the search space is motivated by the residual inverse iteration $t_{RI} = x - T(\sigma)^{-1}T(\theta)x$ (cf. [14]) which converges quickly if σ is close to the wanted eigenvalue. Since in iterative projection methods the new search direction is orthogonalized against the basis of the current search space for stability reasons and since x is already contained in $\mathcal{V}$, the expansion was chosen to be $t_A := T(\sigma)^{-1}T(\theta)x$. In this case we have $|x^H t_{RI}|/\|t_{RI}\| \to 1$ and $x^H t_A/\|t_A\| \to 0$ such that the expansion by t_A turns out to be more robust than the one by t_{RI}.

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