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HOMOGENEOUS JACOBI–DAVIDSON*

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Abstract. We study a homogeneous variant of the Jacobi–Davidson method for the generalized and polynomial eigenvalue problem. While a homogeneous form of these problems was previously considered for the subspace extraction phase, in this paper this form is also exploited for the subspace expansion phase and the projection present in the correction equation. The resulting method can deal with both finite and infinite eigenvalues in a natural and unified way. We show relations with the multihomogeneous Newton method, Rayleigh quotient iteration, and (standard) Jacobi–Davidson for polynomial eigenproblems.

Key words. homogeneous form, quadratic eigenvalue problem, generalized eigenvalue problem, polynomial eigenvalue problem, infinite eigenvalues, correction equation, subspace method, subspace expansion, large sparse matrices, bihomogeneous Newton, multihomogeneous Newton, Rayleigh quotient iteration, Jacobi–Davidson

AMS subject classifications. 65F15, 65F50

1. Introduction. We study a homogeneous Jacobi–Davidson variant for the polynomial eigenproblem

$$P(\lambda)\,\mathbf{x} = (\lambda^m A_m + \lambda^{m-1} A_{m-1} + \cdots + A_0)\,\mathbf{x} = \mathbf{0}, \tag{1.1}$$

where the matrices A_i are (possibly large sparse) $n \times n$ matrices with real or complex entries.

We will focus our discussion on the quadratic eigenvalue problem (QEP)

$$Q(\lambda)\,\mathbf{x} = (\lambda^2 A + \lambda B + C)\,\mathbf{x} = \mathbf{0} \tag{1.2}$$

since it is a nonlinear eigenproblem and it plays an important role in many practical applications (see, e.g., [20]). We will come back to the general problem (1.1) as well as an important special case, the generalized eigenvalue problem

$$A\mathbf{x} = \lambda B\mathbf{x} \tag{1.3}$$

in Sections 4.1 and 4.2.

Since (1.1), (1.2), and (1.3) may have infinite eigenvalues, it is natural to look at the homogeneous form of these problems. Indeed, this form can handle both finite and infinite eigenvalues in a consistent way. Various authors have exploited this form, for instance in the study of for perturbation theory and pseudospectra (see Stewart and Sun [19, Ch. VI], Higham and Tisseur [6], and Dedieu and Tisseur [4]) and in the Jacobi–Davidson (JD) method for the generalized eigenvalue problem (Fokkema, Sleijpen, and Van der Vorst [5]; see also Sleijpen, Booten, Fokkema, and Van der Vorst [16]).

We are interested in subspace methods for the polynomial eigenproblem, which aim at approximating eigenpairs from low-dimensional search spaces. Subspace methods include two important phases: the subspace extraction, where one would like to select approximate

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eigenpairs from a given subspace, and the subspace expansion, where the subspace is enlarged by a new direction to get even better approximations.

While [5] used the homogeneous form for the subspace extraction phase, this paper will exploit this form of the polynomial eigenproblem to propose an alternative Newton or Jacobi–Davidson type *subspace expansion* process. We note that there are also other types of subspace expansion techniques, most notably the second order Arnoldi (SOAR) type method due to Raeven [14] and Bai and Su [2]. It is also natural to exploit the homogenous form for the subspace extraction, see [7] and Section 4.4.

In the next section we will apply Newton to the homogeneous form of (1.2) and derive a new correction equation for Jacobi–Davidson for the quadratic eigenproblem. In Section 3 we will present several alternatives for the projection in the correction equation, and point out relations with the multihomogeneous Newton method. Section 4 discusses some special cases and extensions. Finally, we present numerical experiments and a conclusion in Sections 5 and 6.

2. Subspace expansion for homogeneous Jacobi–Davidson. Let us consider the homogeneous form of (1.2):

$$Q(\alpha_\lambda, \beta_\lambda)\,\mathbf{x} = (\alpha_\lambda^2 A + \alpha_\lambda\beta_\lambda B + \beta_\lambda^2 C)\,\mathbf{x} = \mathbf{0}, \qquad \lambda = \alpha_\lambda/\beta_\lambda.$$

Suppose we have an approximate eigenvector $\mathbf{u} \approx \mathbf{x}$ of unit length and a corresponding approximate eigenvalue $\theta := \alpha/\beta \approx \lambda$ in homogeneous form, where α/β is the Rayleigh quotient of $\mathbf{u}$ and satisfies

$$\mathbf{r} := (\alpha^2 A + \alpha\beta B + \beta^2 C)\,\mathbf{u} \perp \mathbf{u},$$

i.e., it is one of the two solutions of $\alpha^2(\mathbf{u}^*A\mathbf{u}) + \alpha\beta(\mathbf{u}^*B\mathbf{u}) + \beta^2(\mathbf{u}^*C\mathbf{u}) = 0$. The fact that α/β is in homogeneous form means that α and β can still be simultaneously scaled by a nonzero scalar; it is their ratio that matters. An infinite value corresponds to $(\alpha, \beta) = (1, 0)$.

Our main inspiration is formed by the multihomogeneous Newton method, as studied by Dedieu and Shub [3] and Dedieu and Tisseur [4]. We will come back to this method in Section 3.2.

Our *ansatz* is to find an update for both the approximate eigenvalue (in homogeneous form) (α, β) and the approximate eigenvector $\mathbf{u}$: we look for $(\Delta\alpha, \Delta\beta) \perp (\alpha, \beta)$ and $\mathbf{s} \perp \mathbf{u}$ such that

$$\left[(\alpha + \Delta\alpha)^2 A + (\alpha + \Delta\alpha)(\beta + \Delta\beta)B + (\beta + \Delta\beta)^2 C\right](\mathbf{u} + \mathbf{s}) = \mathbf{0}, \tag{2.1}$$

that is, the updated (homogeneous) pair should be an eigenpair, although the updated vector does not have unit length. The appropriate orthogonality condition for $(\Delta\alpha, \Delta\beta)$ is [3, 4]

$$\overline{\alpha}\Delta\alpha + \overline{\beta}\Delta\beta = 0, \tag{2.2}$$

where $\overline{\gamma}$ denotes the complex conjugate of a complex number γ. Discarding the second-order terms in (2.1) we get

$$Q(\alpha, \beta)\,\mathbf{s} = -Q(\alpha, \beta)\,\mathbf{u} - \Delta\alpha(2\alpha A + \beta B)\,\mathbf{u} - \Delta\beta(\alpha B + 2\beta C)\,\mathbf{u}. \tag{2.3}$$

Rather than neglecting the last two terms, we would like to project out these terms, using the relation (2.2). At the same time, we want that the projector preserves the information present in the residual $\mathbf{r}$. These two requirements suggest the oblique projector

$$I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}},$$

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where I is the identity matrix and

$$\mathbf{z} = 2\alpha\overline{\beta}A\mathbf{u} + (|\beta|^2 - |\alpha|^2)B\mathbf{u} - 2\overline{\alpha}\beta C\mathbf{u}; \tag{2.4}$$

here we also need the assumption that $\mathbf{u}^*\mathbf{z} \neq 0$. Projecting (2.3) we get the correction equation

$$\left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right) Q(\alpha,\beta)(I - \mathbf{u}\mathbf{u}^*)\,\mathbf{s} = -Q(\alpha,\beta)\,\mathbf{u}, \qquad \mathbf{s} \perp \mathbf{u}. \tag{2.5}$$

Compared with previous work on the Jacobi–Davidson method for quadratic eigenproblem [16, 18, 21, 9], the correction equation (2.5) is in homogeneous form and has a different projection vector $\mathbf{z}$; see more details in Section 3.1.

Many practical aspects of earlier work (see, e.g., [17]) carry over to the new variant:

- If (2.5) is solved exactly, it has the solution

  $$\mathbf{s} = -\mathbf{u} + \gamma\, Q(\alpha,\beta)^{-1}\mathbf{z}, \tag{2.6}$$

  where $\gamma \in \mathbb{C}$ is such that $\mathbf{s} \perp \mathbf{u}$.
- Instead of an (often expensive) exact solve, we may solve the correction equation approximately, for instance using a few steps of the GMRES method.
- If we have a preconditioner $M \approx Q(\alpha,\beta)$, we may exploit it in solving the correction equation: we use the action of the inverse of

  $$\left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right) M : \mathbf{u}^\perp \to \mathbf{u}^\perp$$

  which is

  $$\left(I - \frac{M^{-1}\mathbf{z}\mathbf{u}^*}{\mathbf{u}^* M^{-1}\mathbf{z}}\right) M^{-1} : \mathbf{u}^\perp \to \mathbf{u}^\perp.$$

  This means that to solve (2.5), we need one action with M^{-1} to precompute $M^{-1}\mathbf{z}$, plus in addition one action per step of the linear solver.
- An "Olsen type" method (see [13] and also [17]) for the QEP would be to take

  $$\widetilde{\mathbf{s}} = -M^{-1}\mathbf{r} + \gamma M^{-1}\mathbf{z},$$

  where $\gamma \in \mathbb{C}$ is such that $\widetilde{\mathbf{s}} \perp \mathbf{u}$.
- It is a sensible idea to solve (2.5) using a Krylov space of the form

  $$\mathcal{K}_m\left(\left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right) Q(\alpha,\beta),\ -\mathbf{r}\right)$$

  since this space is automatically orthogonal to the current approximation $\mathbf{u}$.
- We may be asked to compute eigenvalues close to a target $\tau = \alpha_\tau/\beta_\tau$. In this case, this target is often a better approximate eigenvalue than the Rayleigh quotient in the early stages of the method. Therefore, it may often be favorable in practice to replace the Rayleigh quotient α/β in the left-hand side of (2.5) by the target α_τ/β_τ until the Rayleigh quotient is of sufficient quality (measurable by a small residual norm).

3. Relations. The correction equation (2.5) is closely related to several other methods, as we will now show.

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3.1. Standard Jacobi–Davidson for the quadratic eigenproblem. The standard correction equation of Jacobi–Davidson for the quadratic eigenvalue problem is [16, 18, 21]

$$\left(I - \frac{\mathbf{z}_1\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}_1}\right)(\theta^2 A + \theta B + C)(I - \mathbf{u}\mathbf{u}^*)\,\mathbf{s} = -(\theta^2 A + \theta B + C)\,\mathbf{u}, \qquad \mathbf{s} \perp \mathbf{u},$$

where

$$\mathbf{z}_1 = Q'(\theta)\,\mathbf{u} = (2\theta A + B)\,\mathbf{u}.$$

(See [8] for a derivation; the idea is to project out a multiple of $Q'(\theta)\,\mathbf{u}$, while fixing the residual $Q(\theta)\,\mathbf{u}$.) Switching to homogeneous coordinates we get

$$\mathbf{z}_1 = (2\alpha A + \beta B)\,\mathbf{u} = D_\alpha Q(\alpha, \beta)\,\mathbf{u}, \tag{3.1}$$

where D_α denotes the derivative with respect to α. However, other formulations of the quadratic eigenproblem lead to other projection vectors $\widetilde{\mathbf{z}}$. Suppose for convenience that $\lambda \notin \{0, \infty\}$. Then the formulation $(\lambda A + B + \lambda^{-1} C)\,\mathbf{x} = \mathbf{0}$ leads to the vector

$$\widetilde{\mathbf{z}} = (\theta A - \theta^{-1} C)\,\mathbf{u}, \quad \text{i.e.,} \quad \widetilde{\mathbf{z}} = (\alpha^2 A - \beta^2 C)\,\mathbf{u}. \tag{3.2}$$

Similarly, the formulation $(A + \lambda^{-1} B + \lambda^{-2} C)\,\mathbf{x} = \mathbf{0}$ leads to the vector

$$\mathbf{z}_2 = (\theta B + 2C)\,\mathbf{u}$$

or in homogeneous coordinates

$$\mathbf{z}_2 = (\alpha B + 2\beta C)\,\mathbf{u} = D_\beta Q(\alpha, \beta)\,\mathbf{u}. \tag{3.3}$$

Note that we can also derive this last vector if we consider the *reverse QEP* (which may in particular be attractive if are interested in large and infinite eigenvalues)

$$\lambda^2 Q(\lambda^{-1})\,\mathbf{x} = (A + \lambda B + \lambda^2 C)\,\mathbf{x} = \mathbf{0}.$$

In fact, we can get infinitely many other possibilities for the projection vector $\mathbf{z}$ in a similar way.

The projection vector $\mathbf{z}$ in (2.4) is different in general from the vectors $\mathbf{z}_1$, $\mathbf{z}_2$, and $\widetilde{\mathbf{z}}$ that we have seen in this section. In fact, we have that

$$\mathbf{z} = \overline{\beta}\,\mathbf{z}_1 - \overline{\alpha}\,\mathbf{z}_2 = (\overline{\beta} D_\alpha - \overline{\alpha} D_\beta) Q(\alpha, \beta)\,\mathbf{u}.$$

Therefore the projection vector $\mathbf{z}$ may be interpreted as a mediator between the projection vector $\mathbf{z}_1$ for the eigenvalues around 0 and the projection vector $\mathbf{z}_2$ for the eigenvalues around ∞. In particular, (2.4) is equal to $\mathbf{z}_1$ in $\theta = 0$ and equal to $\mathbf{z}_2$ in $\theta = \infty$.

3.2. Multihomogeneous Newton. We now focus on the multihomogeneous Newton as studied by Dedieu and Shub [3] and Dedieu and Tisseur [4]. They show that the updates $(\Delta\alpha, \Delta\beta)$ and $\mathbf{s}$ should satisfy the system

$$\begin{bmatrix} Q(\alpha, \beta) & (2\alpha A + \beta B)\,\mathbf{u} & (\alpha B + 2\beta C)\,\mathbf{u} \\ \mathbf{u}^* & 0 & 0 \\ \mathbf{0}^* & \overline{\alpha} & \overline{\beta} \end{bmatrix} \begin{bmatrix} \mathbf{s} \\ \Delta\alpha \\ \Delta\beta \end{bmatrix} = - \begin{bmatrix} Q(\alpha, \beta)\,\mathbf{u} \\ 0 \\ 0 \end{bmatrix}. \tag{3.4}$$

We now show that this system is equivalent to the correction equation (2.5) with $\mathbf{z}$ as in (2.4) (cf. [16, Thm. 3.5]).

PROPOSITION 3.1. *Let* $\mathbf{u}$ *be an approximate eigenvector and let* α/β *be the Rayleigh quotient of* $\mathbf{u}$ *(which implies* $Q(\alpha,\beta)\,\mathbf{u} \perp \mathbf{u}$*). Then (2.5) is equivalent to (3.4) in the following sense: if* $(\mathbf{s}, \Delta\alpha, \Delta\beta)$ *is a solution to (3.4), then* $\mathbf{s}$ *is a solution to (2.5), and if* $\mathbf{s}$ *is a solution to (2.5), then there exist* $\Delta\alpha$ *and* $\Delta\beta$ *such that* $(\mathbf{s}, \Delta\alpha, \Delta\beta)$ *is a solution to (3.4).*

Proof. If $(\mathbf{s}, \Delta\alpha, \Delta\beta)$ is a solution to (3.4), then from (2.3) and (2.2) we see that $\mathbf{s}$ is a solution to (2.5). On the other hand, if $\mathbf{s}$ is a solution to (2.5), then there exists a $\gamma \in \mathbb{C}$ such that $Q(\alpha,\beta)\,\mathbf{s} = -Q(\alpha,\beta)\,\mathbf{u} + \gamma\mathbf{z}$, where $\mathbf{z}$ is as in (2.4). Now we realize that $\mathbf{z} = \overline{\beta}\,\mathbf{z}_1 - \overline{\alpha}\,\mathbf{z}_2$, where $\mathbf{z}_1$ and $\mathbf{z}_2$ are as in (3.1) and (3.3). Hence, the result now follows from taking $\Delta\alpha = -\gamma\overline{\beta}$ and $\Delta\beta = \gamma\overline{\alpha}$. □

In [3] and [4], (3.4) is derived by a Newton process on the space $S^{n-1} \times \mathbb{P}$, where $S^{n-1} = \{\mathbf{x} \in \mathbb{C}^n : \|\mathbf{x}\| = 1\}$ is the unit sphere, $\mathbb{P}$ is the one-dimensional projective space over $\mathbb{C}$, and $\|\cdot\|$ is the two-norm. We note that we can also derive (3.4) in an alternative, slightly easier way as follows.

Let $\mathbf{a} \in \mathbb{C}^n$ and $(\gamma, \delta) \in \mathbb{P}$ be fixed scaling quantities in the equations

$$\begin{aligned}(\alpha^2 A + \alpha\beta B + \beta^2 C)\,\mathbf{x} &= \mathbf{0},\\ \mathbf{a}^*\mathbf{x} - 1 &= 0,\\ \overline{\gamma}\alpha + \overline{\delta}\beta - 1 &= 0.\end{aligned}$$

One may check that we get (3.4) when we write down the Newton correction for this system of equations and subsequently replace the "scaling quantities" (γ, δ) and $\mathbf{a}$ by the current iterates (α, β) and $\mathbf{u}$, respectively.

In particular, since this approach is a Newton method, we get asymptotic quadratic convergence if the Jacobian is asymptotically nonsingular (cf. also [9]).

PROPOSITION 3.2. *Suppose the homogeneous Jacobi–Davidson method, where the correction equations (2.5) are solved exactly, converges to a simple eigenvalue, with right and left eigenvectors* $\mathbf{x}$ *and* $\mathbf{y}$*, respectively. Let* $\mathbf{z}_\infty$ *be the "asymptotic* $\mathbf{z}$ *vector",* $\mathbf{z}_\infty = (\overline{\beta}D_\alpha - \overline{\alpha}D_\beta)Q(\alpha,\beta)\,\mathbf{x}$*. Assume that* $\mathbf{x}^*\mathbf{z}_\infty \neq 0$ *and* $\mathbf{y}^*\mathbf{z}_\infty \neq 0$*. Then the asymptotic convergence is quadratic.*

Proof. Because the homogeneous JD method is a Newton method, we only have to show that the "asymptotic Jacobian"

$$\left(I - \frac{\mathbf{z}_\infty \mathbf{x}^*}{\mathbf{x}^*\mathbf{z}_\infty}\right) Q(\alpha,\beta) : \mathbf{x}^\perp \to \mathbf{x}^\perp \tag{3.5}$$

is nonsingular. Suppose

$$\left(I - \frac{\mathbf{z}_\infty \mathbf{x}^*}{\mathbf{x}^*\mathbf{z}_\infty}\right) Q(\alpha,\beta)\,\mathbf{s} = \mathbf{0}$$

for an $\mathbf{s} \perp \mathbf{x}$. Then there exists a $\xi \in \mathbb{C}$ such that

$$Q(\alpha,\beta)\,\mathbf{s} = \xi\,\mathbf{z}_\infty.$$

Since (α,β) is supposed to be simple, there exists a unique left eigenvector $\mathbf{y}$ such that $0 = \mathbf{y}^*Q(\alpha,\beta)\,\mathbf{s} = \xi\,\mathbf{y}^*\mathbf{z}_\infty$. Because of the assumption that $\mathbf{y}^*\mathbf{z}_\infty \neq 0$, we must have $\xi = 0$ and this implies that the operator (3.5) is injective and hence bijective. □

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3.3. Homogeneous Rayleigh quotient iteration. First recall that a step of Rayleigh quotient iteration (RQI) for the standard eigenproblem $A\mathbf{x} = \lambda\mathbf{x}$ is to solve $\widetilde{\mathbf{u}}$ from $(A - \theta I)\,\widetilde{\mathbf{u}} = \mathbf{u}$, where $(\theta, \mathbf{u})$ is the current approximate eigenpair. For the general polynomial eigenvalue problem a generalization of RQI is less well known. For a derivation, we start with

$$\mathbf{0} = Q(\lambda)\,\mathbf{x} = Q(\theta)\,\mathbf{x} + (Q(\lambda) - Q(\theta))\,\mathbf{x} \approx Q(\theta)\,\mathbf{x} + (\lambda - \theta)\,Q'(\theta)\,\mathbf{x}.$$

Therefore, inspired by $Q(\theta)^{-1}Q'(\theta)\,\mathbf{x} \approx (\lambda - \theta)^{-1}\mathbf{x}$, a step of Rayleigh quotient iteration for the polynomial eigenproblem is to solve $\widetilde{\mathbf{u}}$ from (cf., e.g., [20])

$$Q(\theta)\,\widetilde{\mathbf{u}} = Q'(\theta)\,\mathbf{u}. \tag{3.6}$$

Let us now consider a generalization of the RQI method for homogeneous polynomial eigenvalue problem, where again we will use the quadratic eigenproblem as a role model. We have

$$\begin{aligned}\mathbf{0} &= Q(\alpha_\lambda, \beta_\lambda)\,\mathbf{x} = Q(\alpha, \beta)\,\mathbf{x} + (Q(\alpha_\lambda, \beta_\lambda) - Q(\alpha, \beta))\,\mathbf{x}\\ &\approx Q(\alpha, \beta)\,\mathbf{x} + ((\alpha_\lambda - \alpha)D_\alpha + (\beta_\lambda - \alpha)D_\beta)\,Q(\alpha, \beta)\,\mathbf{x}.\end{aligned}$$

At this point we use the orthogonality condition (2.2), so that a step of homogeneous Rayleigh quotient for the polynomial eigenproblem is to solve $\widetilde{\mathbf{u}}$ from

$$Q(\alpha, \beta)\,\widetilde{\mathbf{u}} = (\overline{\beta}D_\alpha - \overline{\alpha}D_\beta)\,Q(\alpha, \beta)\,\mathbf{u} = \mathbf{z}. \tag{3.7}$$

Comparing this with the exact solution (2.6) to the correction equation (2.5), we see that an exact step of (homogeneous) RQI for the QEP is equivalent to an exact step of (homogeneous) JD for the QEP, in the sense that $\widetilde{\mathbf{u}}$ in (3.6) is a multiple of $\mathbf{u} + \mathbf{s}$ in (2.6).

However, we will usually solve (2.5) and (3.7) inexactly in practice. If we solve (3.7) by a Krylov subspace method, we look for an approximation to $\widetilde{\mathbf{u}}$ in the Krylov search space

$$\mathcal{K}_l(Q(\alpha, \beta), \mathbf{z})$$

for an (often) low dimension l. An important observation is that $\mathbf{u}$ will generally not be in this search space. If $\mathbf{u}$ is already an approximation of good quality, this unfortunate fact makes Rayleigh quotient iteration for polynomial eigenproblems of large size less attractive (similar remarks hold for "non-homogeneous RQI" (3.6)).

In contrast, the homogeneous JD method looks for an *update* to the approximate vector $\mathbf{u}$, rather than directly for a new approximate vector $\widetilde{\mathbf{u}}$, and therefore does not share the above problem and may as a result be more attractive. We note that this situation is somewhat similar to issues one faces when using preconditioning for RQI in the standard eigenvalue problem, see [15].

4. Extensions and special cases. In this section, we will extend the multihomogeneous Newton approach, or homogenous Jacobi–Davidson technique, to general polynomial eigenvalue problems. Then we will briefly study the special important case of the generalized eigenproblem and summarize some results concerning homogeneous subspace *extraction* from [7].

4.1. The polynomial eigenproblem. The Jacobi–Davidson method has also been exploited for polynomial eigenproblems of which the polynomial is of degree > 2, for instance cubic [10, 11], quartic, or quintic [12]; see also [22] and the references therein. The multihomogeneous Newton, or homogeneous JD expansion, technique can be generalized to the

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general polynomial eigenvalue problem as follows. Consider the homogeneous version of the polynomial eigenproblem (1.1):

$$P(\alpha_\lambda, \beta_\lambda)\,\mathbf{x} = (\alpha_\lambda^m A_m + \alpha_\lambda^{m-1}\beta_\lambda A_{m-1} + \cdots + \alpha_\lambda \beta_\lambda^{m-1} A_1 + \beta_\lambda^m A_0)\,\mathbf{x} = \mathbf{0}.$$

Let $(\alpha/\beta, \mathbf{u})$ an approximate eigenpair with $P(\alpha,\beta)\,\mathbf{u} \perp \mathbf{u}$. With the *ansatz*

$$P((\alpha + \Delta\alpha), (\beta + \Delta\beta))(\mathbf{u} + \mathbf{s}) = \mathbf{0},$$

where $\mathbf{s} \perp \mathbf{u}$ and $\overline{\alpha}\Delta\alpha + \overline{\beta}\Delta\beta = 0$, we have the first order approximation

$$P(\alpha,\beta)\,\mathbf{s} = -P(\alpha,\beta)\,\mathbf{u} - \Delta\alpha\, D_\alpha P(\alpha,\beta)\,\mathbf{u} - \Delta\beta\, D_\beta P(\alpha,\beta)\,\mathbf{u}.$$

Using (2.2), and projecting out the resulting vector, the correction equation becomes

$$\left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right) P(\alpha,\beta)(I - \mathbf{u}\mathbf{u}^*)\,\mathbf{s} = -P(\alpha,\beta)\,\mathbf{u},$$

where

$$\mathbf{z} = (\overline{\beta} D_\alpha - \overline{\alpha} D_\beta) P(\alpha,\beta)\,\mathbf{u}. \tag{4.1}$$

Note that earlier work on JD for the polynomial eigenproblem [16, 18, 21, 1, 9] suggested the projection vector

$$\mathbf{z}_1 = P'(\theta)\,\mathbf{u} = (m\theta^{m-1} A_m + (m-1)\,\theta^{m-2} A_{m-1} + \cdots + A_1)\,\mathbf{u}.$$

As for the quadratic eigenproblem, the projection vector $\mathbf{z}$ is a linear combination of the vector $\mathbf{z}_1$ in homogeneous coordinates

$$\mathbf{z}_1 = (m\alpha^{m-1} A_m + (m-1)\,\alpha^{m-2}\beta A_{m-1} + \cdots + \beta^{m-1} A_1)\,\mathbf{u} = D_\alpha P(\alpha,\beta)\,\mathbf{u}$$

and the vector

$$\mathbf{z}_2 = (\alpha^{m-1} A_{m-1} + \cdots + (m-1)\,\alpha\beta^{m-2} A_1 + m\beta^{m-1} A_0)\,\mathbf{u} = D_\beta P(\alpha,\beta)\,\mathbf{u}.$$

This $\mathbf{z}_2$ is the homogeneous version of

$$(A_{m-1} + 2\lambda A_{m-1} + \cdots + (m-1)\,\lambda^{m-2} A_1 + m\lambda^{m-1} A_0)\,\mathbf{u},$$

which can be derived from the reverse polynomial eigenproblem

$$\lambda^m P(\lambda^{-1}) = (A_m + \lambda A_{m-1} + \cdots + \lambda^{m-1} A_1 + \lambda^m A_0)\,\mathbf{x} = \mathbf{0}.$$

As for the QEP, we have the relation $\mathbf{z} = \overline{\beta}\,\mathbf{z}_1 - \overline{\alpha}\,\mathbf{z}_2$ for the general polynomial eigenproblem.

4.2. The generalized eigenproblem. Let us briefly study the homogeneous Jacobi–Davidson method for the generalized eigenvalue problem

$$A\mathbf{x} = \lambda B\mathbf{x}, \qquad (\beta_\lambda A - \alpha_\lambda B)\,\mathbf{x} = \mathbf{0}$$

since this is an important problem in many applications. Let $(\alpha/\beta, \mathbf{u})$ be an approximate eigenpair. The homogeneous form of the correction equation is

$$\left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right)(\beta A - \alpha B)(I - \mathbf{u}\mathbf{u}^*)\,\mathbf{s} = -(\beta A - \alpha B)\,\mathbf{u}, \qquad \mathbf{s} \perp \mathbf{u},$$

where the projection vector is

$$\mathbf{z} = \overline{\alpha} A\mathbf{u} + \overline{\beta} B\mathbf{u}.$$

In [16, Thm. 3.2] it was proved that with a choice for the projection vector of any linear combination of $A\mathbf{u}$ and $B\mathbf{u}$ we get asymptotically quadratic convergence if the correction equations are solved exactly. Remarkably, to optimally expand the test space, with only the target as a priori information, the combination $\overline{\alpha}_\tau A\mathbf{u} + \overline{\beta}_\tau B\mathbf{u}$ was suggested for the JDQZ type method in [5].

4.3. Two-sided variant. We remark that a homogeneous approach is also possible in combination with a two-sided method. Let us again consider the QEP. In a two-sided JD variant we have two search spaces, $\mathcal{U}$ for the (right) eigenvector $\mathbf{x}$, and $\mathcal{V}$ for the left eigenvector $\mathbf{y}$ (satisfying $\mathbf{y}^* Q(\alpha_\lambda, \beta_\lambda) = \mathbf{0}^*$).

If we have an approximation $(\alpha/\beta, \mathbf{u}, \mathbf{v}) \approx (\alpha_\lambda/\beta_\lambda, \mathbf{x}, \mathbf{y})$, where $\mathbf{v}^* Q(\alpha, \beta)\, \mathbf{u} = 0$, then the correction equation for $\mathbf{u}$ takes the form

$$\left(I - \frac{\mathbf{z}\mathbf{v}^*}{\mathbf{v}^*\mathbf{z}}\right) Q(\alpha, \beta)\, \mathbf{s} = -Q(\alpha, \beta)\, \mathbf{u}.$$

Here $\mathbf{z}$ is as in (4.1); one option is to look for a bi-orthogonal update, $\mathbf{s} \perp \mathbf{v}$ for $\mathbf{u}$. Similarly, the equation for a correction $\mathbf{t}$ for $\mathbf{v}$ is of the form

$$\left(I - \frac{\mathbf{w}\mathbf{u}^*}{\mathbf{u}^*\mathbf{w}}\right) (Q(\alpha, \beta))^* \mathbf{t} = -(Q(\alpha, \beta))^*\, \mathbf{v}.$$

where $\mathbf{w} = ((\overline{\beta} D_\alpha - \overline{\alpha} D_\beta) Q(\alpha, \beta))^*\, \mathbf{v}$.

4.4. Homogeneous subspace extraction methods. In [7] it is shown that the homogeneous form for the polynomial eigenvalue problem can also be used in the subspace extraction phase. We now summarize a few results.

Let $\mathcal{U} = \mathcal{U}_k$ be a (low) k-dimensional search space. We are looking for an approximate eigenpair $(\theta, \mathbf{u}) \approx (\lambda, \mathbf{x})$ where $\mathbf{u} \in \mathcal{U}$, so we can write $\mathbf{u} = U_k \mathbf{c}$, where the columns of U_k form an orthonormal basis for $\mathcal{U}_k$ and $\mathbf{c} \in \mathbb{C}^k$ has unit norm. The standard extraction to determine approximate pairs from the Galerkin condition $Q(\theta)\, \mathbf{u} \perp \mathcal{U}$ straightforwardly translates to its homogeneous form

$$U_k^* Q(\alpha, \beta) U_k \mathbf{c} = \mathbf{0}.$$

For eigenpairs close to a target $(\alpha_\tau, \beta_\tau)$, the standard extraction is often not optimal and a harmonic or refined approach is recommended [9]. The counterpart of the harmonic extraction $Q(\theta)\, \mathbf{u} \perp Q(\tau)\mathcal{U}$ (see [9]) is to determine candidate approximate eigenpairs $(\alpha/\beta, \mathbf{u})$ from

$$Q(\alpha, \beta) U_k\, \mathbf{c} \perp Q(\alpha_\tau, \beta_\tau) \mathcal{U}.$$

Finally, the refined extraction determines an approximate eigenvector as a minimizing argument of the expression

$$\min_{\mathbf{u} \in \mathcal{U},\ \|\mathbf{u}\|=1} \|Q(\alpha_\tau, \beta_\tau)\, \mathbf{u}\| = U_k \cdot \min_{\mathbf{c} \in \mathbb{C}^k,\ \|\mathbf{c}\|=1} \|Q(\alpha_\tau, \beta_\tau) U_k\, \mathbf{c}\|.$$

For more details we refer to [7].

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Algorithm 1 Homogeneous Jacobi–Davidson for the polynomial eigenvalue problem

Input: A device to compute $A_j\mathbf{x}$ for arbitrary $\mathbf{x}$, a starting vector $\mathbf{u}_1$, a target τ, a tolerance ε, and a parameter `threshold`

Output: An approximate eigenpair $(\alpha/\beta, \mathbf{u})$ with $\alpha/\beta \approx \tau$

1: $\mathbf{s} = \mathbf{u}_1$
2: **for** $k = 1, 2, \ldots$ **do**
3: $\quad \mathtt{rgs}(U_{k-1}, \mathbf{s}) \to U_k$
4: $\quad$ Perform a homogenous extraction process (see Section 4.4) to get $(\alpha/\beta, \mathbf{c})$, where $\alpha/\beta \approx \tau$
5: $\quad \mathbf{u} = U_k\mathbf{c}$
6: $\quad \mathbf{r} = P(\alpha, \beta)\,\mathbf{u}$
7: $\quad$ Stop if $\|\mathbf{r}\| \le \varepsilon$
8: $\quad$ Solve (approximately) an $\mathbf{s} \perp \mathbf{u}$ from one of the following equations:
9: $\quad \left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right) P(\alpha, \beta)\,\mathbf{s} = -\mathbf{r}, \qquad \mathbf{z} = (\overline{\beta} D_\alpha - \overline{\alpha} D_\beta) P(\alpha, \beta)\,\mathbf{u},$ (if $\|\mathbf{r}\| \le$ `threshold`)
10: $\quad \left(I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}\right) P(\alpha_\tau, \beta_\tau)\,\mathbf{s} = -\mathbf{r}, \qquad \mathbf{z} = (\overline{\beta}_\tau D_\alpha - \overline{\alpha}_\tau D_\beta) P(\alpha_\tau, \beta_\tau)\,\mathbf{u}$ (if $\|\mathbf{r}\| >$ `threshold`)
11: **end for**

5. Numerical experiments. For completeness and convenience, we first give pseudocode for the homogeneous JD method; see [9] for its non-homogeneous counterpart.

The "`rgs`" in Line 3 stands for repeated Gram–Schmidt or any other numerical stable way to form an orthonormal basis for the search space. For simplicity, we have omitted a restart procedure.

EXPERIMENT 5.1. In our first example, A is a diagonal matrix with entries 0, …, 999, $B = i \cdot I$, and $C = I$. We run the homogeneous JD method to find the absolute largest eigenvalue, with a set of 10 different random starting vectors. The method correctly finds $\lambda = \infty$ (or $\lambda = 1/\beta$ for a very small $|\beta|$) in all cases in an average 22 iterations. For comparison: it finds the eigenvalue closest to target $\tau = 0$, $\lambda \approx 0.03i$ in 51 iterations on average, although it must be noted that this eigenvalue is somewhat more "interior" than the infinite eigenvalue.

Also from several other unreported experiments with quadratic eigenvalue problems with singular A matrix having infinite eigenvalues, we conclude that the homogeneous JD indeed finds infinite eigenvalues with no more effort than finite ones (cf. also similar similar remarks in [4] about the homogeneous Newton method).

The standard JD variant is unsuited to compute both finite and infinite eigenvalues in one consistent procedure. Therefore, we perform some experiments comparing the methods with different projection vectors for finding *finite* eigenvalues.

We compare the homogeneous Jacobi–Davidson method described in Algorithm 1 with the standard version in [9] (see also [16, 18, 21]) and some other alternative variants. The choices for the methods are the following: we use the standard extraction process; the minimum and maximum dimensions of the search space are 10 and 30, respectively; the tolerance is 10^{-6} times the matrix one-norm; the correction equations are solved by 10 steps of the GMRES method; and the maximum number of outer iterations is 200.

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EXPERIMENT 5.2. For the second example we take `utrecht-1331`, a 1331×1331 QEP, where A and C are symmetric positive definite, and B is complex, singular, and non-Hermitian; see also [2, Ex. 4]. We try to compute the eigenpair closest to target $\tau = -5$. The two closest eigenvalues are $\lambda_1 \approx -0.0003 + 0.0026i$ and $\lambda_2 \approx -5.2 - 49.5i$, which are relatively clustered compared to the largest eigenvalue $\approx -195 - 4314i$; see Figure 5.1 for the spectrum.

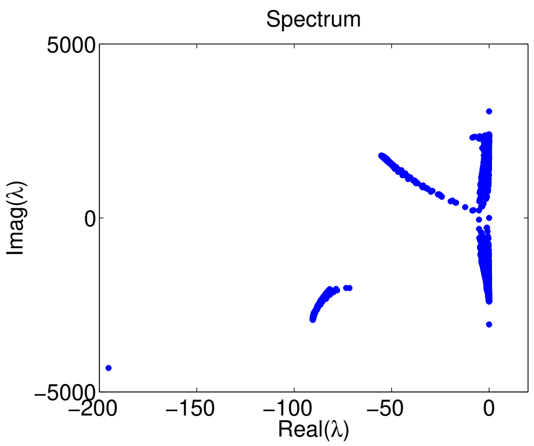

FIG. 5.1. *Spectrum of the* `utrecht-1331` *problem.*

For Table 5.1 we take 5 different projection vectors $\mathbf{z}$ in the left projection $I - \frac{\mathbf{z}\mathbf{u}^*}{\mathbf{u}^*\mathbf{z}}$ in the correction equation (2.5): the standard choice $\mathbf{z}_1 = Q'(\theta)\,\mathbf{u} = (2\theta A + B)\,\mathbf{u}$ (see (3.1)); the two alternative presented in Section 3.1: $\widetilde{\mathbf{z}} = (\theta A - \theta^{-1} C)\,\mathbf{u}$ (see (3.2)) and $\mathbf{z}_2 = (\theta B + 2C)\,\mathbf{u}$ (see (3.3)); the homogeneous vector $\mathbf{z} = (\overline{\beta} D_\alpha - \overline{\alpha} D_\beta)\, Q(\alpha,\beta)\,\mathbf{u}$ (see (2.4)) in standard coordinates:

$$\mathbf{z} = 2\theta A\mathbf{u} + (1 - |\theta|^2)B\mathbf{u} - 2\overline{\theta}C\mathbf{u}$$

and the vector $\mathbf{u}$ yielding an orthogonal projection. We would like to stress that the last choice has no mathematical justification in the sense that with this projection one cannot expect asymptotically quadratic convergence in general (if the correction equations would be solved exactly).

TABLE 5.1
Average number of outer iterations (out of 10 cases) for the JD method for different projection vectors and the `utrecht-1331` *test problem.*

Projection vector		Iterations
Standard	$\mathbf{z}_1 = Q'(\theta)\,\mathbf{u} = (2\theta A + B)\,\mathbf{u}$ (see (3.1))	18.4
	$\widetilde{\mathbf{z}} = (\theta A - \theta^{-1} C)\,\mathbf{u}$ (see (3.2))	16.9
	$\mathbf{z}_2 = (\theta B + 2C)\,\mathbf{u}$ (see (3.3))	16.6
Homogeneous	$\mathbf{z} = (\overline{\beta} D_\alpha - \overline{\alpha} D_\beta)\, Q(\alpha,\beta)\,\mathbf{u}$	16.6
Orthogonal	$\mathbf{u}$	16.5

Again, we take a set of 10 random starting vectors and we average the necessary number of outer iterations. From the results in Table 5.1 we see that although the iteration numbers are relatively similar, the standard JD approach is the slowest. Surprisingly, the orthogonal projection vector $\mathbf{u}$ is the (slight) winner; this suggest that taking orthogonal updates throughout the process (which can be thought of as an "optimal expansion"), makes up for the lack of an asymptotically optimal convergence.

We would like to mention that we repeated Experiment 5.2 for many other test matrices using the standard extraction and different projection vectors; the results were roughly comparable in every case.

In the correction equation, we have to (approximately) solve linear systems with the operator that ultimately (upon convergence to an eigenpair $(\lambda, \mathbf{x})$) becomes

$$\left(I - \frac{\mathbf{z}_\infty \mathbf{x}^*}{\mathbf{x}^* \mathbf{z}_\infty}\right) Q(\alpha, \beta)(I - \mathbf{x}\mathbf{x}^*) : \mathbf{x}^\perp \to \mathbf{x}^\perp.$$

For this reason, it is interesting to compare the asymptotic effective condition number of this operator for the different options for $\mathbf{z}_\infty$: $(2\lambda A + B)\,\mathbf{x}$, $(\lambda A - \lambda^{-1} C)\,\mathbf{x}$, $(\lambda B + 2C)\,\mathbf{x}$, $(2\lambda A + (1 - |\lambda|^2)B - 2\overline{\lambda}C)\,\mathbf{x}$, and $\mathbf{x}$, respectively. (By the effective condition number we mean the condition of the operator seen as a map from $\mathbf{x}^\perp$ to $\mathbf{x}^\perp$.) However, a conclusion from unreported experiments is that, apart from the orthogonal choice $\mathbf{z} = \mathbf{x}$, every other choice for $\mathbf{z}$ gives rise to both the best condition number in some cases, but the worst in other cases; no general pattern could be discovered.

6. Conclusions. We presented a homogeneous version of Jacobi–Davidson for the generalized, quadratic, and general polynomial eigenproblem. This approach is inspired by the multihomogeneous Newton approach as described by Dedieu and Shub [3] and Dedieu and Tisseur [4].

The main advantage of the homogeneous approach is that it allows us to treat finite and infinite eigenvalues of a polynomial eigenvalue problem in a natural and equal way, without having to switch from one representation of a polynomial eigenproblem to another. The new variant can be easily implemented (existing non-homogeneous codes only require minor changes) with exactly the same computational costs and storage requirements.

We compared the new method with "standard" JD as well as (homogeneous) RQI for the polynomial problem. We have argued that, when for large problems the inner equations are solved inexactly, one has good reasons to prefer JD over RQI. In several experiments for *finite* eigenvalues, the homogeneous JD method performed equal or somewhat better than its non-homogeneous counterpart. The main surprise here, however, is the surprisingly good results obtained by the variant with the orthogonal projection, which, although without "asymptotic justification", seems to have enough practical advantages such as orthogonal updates and a well-conditioned correction equation.

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