

# Utilizing an invariance of Krylov subspaces with the Jacobi–Davidson method for eigenvalue problems

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## 1 Introduction

We consider computing a few eigenpairs  $(\lambda, \mathbf{x})$  of an  $n \times n$  matrix  $A$ , i.e., the standard eigenvalue problem

$$A\mathbf{x} = \lambda\mathbf{x} \quad (\mathbf{x} \neq \mathbf{0}). \quad (1)$$

The Jacobi–Davidson (JD) method [6, 2, 1] is an iterative method for the problem and has attracted much attention [3]. Suppose a subspace is generated, and an approximate eigenpair is given by using the subspace. Then, the JD method searches for a correction vector which corrects the approximate eigenvector to expand the subspace. If the subspace is expanded by the exact correction vector, then an eigenvector will be in the expanded subspace. Hence, what is important in practical computation is how to compute an approximate correction vector, by which the subspace is expanded.

The correction vector is a solution of an equation which contains a wanted eigenvalue [6]. Usually [6, 2], the eigenvalue in the equation is replaced by its approximation, e.g., the approximate eigenvalue generated by using the subspace. As a result, a linear equation is derived, which is called a correction equation. In this way, the correction equation is determined by the approximate eigenvalue. If the correction equation contains a well approximated eigenvalue, then its solution can be suitable to expand the subspace [2]. Finally, the correction equation is approximately solved by, e.g., a few steps of GMRES [5], and then an approximate solution is used to expand the subspace.

In this report, we consider another approach to the correction vector by utilizing an invariance of Krylov subspaces. The invariance enables us to use one Krylov subspace for two aims. The first aim is to compute approximate eigenvalues that determine correction equations. The second aim is to solve the equations approximately. By the choice of a correction equation and its approximate solution, we propose a new version of the JD method.

The rest of this report is organized as follows. In §2, we introduce the JD method. In §3, we consider utilizing an invariance of Krylov subspaces, and

derive a new version of the JD method. To show the convergence behavior of the methods, we report some numerical experiments in §4. Finally, we summarize the report in §5.

Throughout the paper, the  $n \times n$  identity matrix is denoted by  $I$ . The transpose and conjugate transpose are denoted by the superscripts  $(\cdot)^T$  and  $(\cdot)^*$ , respectively. The  $m$  dimensional Krylov subspace with respect to  $A$  and a vector  $\mathbf{v}$ ,  $\text{span}\{\mathbf{v}, A\mathbf{v}, \dots, A^{m-1}\mathbf{v}\}$ , is denoted by  $\mathcal{K}_m(A, \mathbf{v})$ . The 2-norm is denoted by  $\|\cdot\|$ . For subspaces  $\mathcal{S}_1$  and  $\mathcal{S}_2$ , the direct sum of  $\mathcal{S}_1$  and  $\mathcal{S}_2$ ,  $\text{span}\{\mathbf{s}_1 + \mathbf{s}_2 \mid \mathbf{s}_i \in \mathcal{S}_i, i = 1, 2\}$ , is denoted by  $\mathcal{S}_1 \oplus \mathcal{S}_2$ . In the case of  $\mathcal{S}_1 \perp \mathcal{S}_2$ ,  $\mathcal{S}_1 \oplus \mathcal{S}_2$  is especially denoted by  $\mathcal{S}_1 \odot \mathcal{S}_2$ . The complementary projector of  $\mathbf{v}$  for  $\|\mathbf{v}\| = 1$  is defined by  $I - \mathbf{v}\mathbf{v}^*$  and is denoted by  $P_{\perp\mathbf{v}}$ .

## 2 The JD method

Suppose a subspace  $\mathcal{Q}_k$  is generated at the  $k$ th iteration in the JD method, and an approximation  $(\theta^{(k)}, \mathbf{u}^{(k)})$  of a wanted eigenpair  $(\lambda, \mathbf{x})$  is produced by using  $\mathcal{Q}_k$ . Here,  $\|\mathbf{u}^{(k)}\| = 1$  and  $\theta^{(k)} := (\mathbf{u}^{(k)})^* A \mathbf{u}^{(k)}$ . The residual vector is defined by  $\mathbf{r}^{(k)} := A \mathbf{u}^{(k)} - \theta^{(k)} \mathbf{u}^{(k)}$ . If the residual norm  $\|\mathbf{r}^{(k)}\|$  is enough small, the iteration is stopped. Otherwise, the subspace will be expanded for a better approximated eigenpair. Here, we describe how to generate a next basis vector to expand the subspace.

The JD method [6] is based on the Jacobi's idea [4] that is to find a correction vector  $\mathbf{t} := \mathbf{x} - \mathbf{u}^{(k)}$  satisfying the orthogonality  $\mathbf{t} \perp \mathbf{u}^{(k)}$ . Since the eigenvector  $\mathbf{x}$  will be found in a subspace  $\mathcal{Q}_k \oplus \text{span}\{\mathbf{t}\}$ , the JD method searches for the correction vector  $\mathbf{t}$  to expand the subspace  $\mathcal{Q}_k$ . By (1),  $\mathbf{t}$  satisfies

$$A(\mathbf{u}^{(k)} + \mathbf{t}) = \lambda(\mathbf{u}^{(k)} + \mathbf{t}). \quad (2)$$

From (2), it follows that  $(A - \lambda I)\mathbf{t} = -\mathbf{r}^{(k)} + (\lambda - \theta^{(k)})\mathbf{u}^{(k)}$ . Multiplying the both sides in this equation by  $P_{\perp\mathbf{u}^{(k)}}$  results in  $P_{\perp\mathbf{u}^{(k)}}(A - \lambda I)\mathbf{t} = -\mathbf{r}^{(k)}$ . Since  $\mathbf{t} \perp \mathbf{u}^{(k)}$ , we have

$$P_{\perp\mathbf{u}^{(k)}}(A - \lambda I)P_{\perp\mathbf{u}^{(k)}}\mathbf{t} = -\mathbf{r}^{(k)}. \quad (3)$$

If the unknown eigenvalue  $\lambda$  in (3) is replaced by its approximation  $\theta^{(k)}$ , while keeping the orthogonality to  $\mathbf{u}^{(k)}$ , then we reach a correction equation [6]:

$$P_{\perp\mathbf{u}^{(k)}}(A - \theta^{(k)}I)P_{\perp\mathbf{u}^{(k)}}\mathbf{t}_{\text{JD}} = -\mathbf{r}^{(k)}, \quad (4)$$

where  $\mathbf{t}_{\text{JD}} \perp \mathbf{u}^{(k)}$ . If  $\theta^{(k)}$  is a good approximation of  $\lambda$ , an approximate correction vector will be produced by solving the linear equation (4).

To compute the correction vector, it was proposed in [6] that (4) is approximately solved by an iterative method, e.g., a few steps of GMRES [5].

Finally, an approximate solution of (4) is orthonormalized against the basis of  $\mathcal{Q}_k$ , and then the resulting vector is the next basis vector to expand  $\mathcal{Q}_k$ .

### 3 New approach to the correction vector

We show a decomposition of a Krylov subspace with respect to  $A$  and a vector  $\mathbf{v}$  with  $\|\mathbf{v}\| = 1$  for any  $\gamma \in \mathbb{C}$ :

$$\mathcal{K}_m(A, \mathbf{v}) = \text{span}\{\mathbf{v}\} \odot \mathcal{K}_{m-1}(P_{\perp\mathbf{v}}(A - \gamma I)P_{\perp\mathbf{v}}, P_{\perp\mathbf{v}}A\mathbf{v}). \quad (5)$$

We will utilize (5) to compute the correction vector approximately for alternative expansion of the subspace  $\mathcal{Q}_k$ .

As supposed in §2, the approximate eigenpair  $(\theta^{(k)}, \mathbf{u}^{(k)})$  is given by using the subspace  $\mathcal{Q}_k$ . For the correction vector, we consider solving a linear equation

$$P_{\perp\mathbf{u}^{(k)}}(A - \gamma^{(k)}I)P_{\perp\mathbf{u}^{(k)}}\mathbf{t}_* = -\mathbf{r}^{(k)}, \quad (6)$$

where  $\mathbf{t}_* \perp \mathbf{u}^{(k)}$  and  $\gamma^{(k)} \in \mathbb{C}$  is undetermined. As we have reviewed the JD method in §2, it is appropriate to solve (6) after setting  $\gamma^{(k)}$  to a well approximated eigenvalue. To this end, let us utilize (5) for  $\gamma = \gamma^{(k)}$  and  $\mathbf{v} = \mathbf{u}^{(k)}$ ; hence,  $P_{\perp\mathbf{v}}A\mathbf{v} = \mathbf{r}^{(k)}$ . If we generate a Krylov subspace  $\mathcal{K}_m(A, \mathbf{u}^{(k)})$ , then we also have a Krylov subspace  $\mathcal{K}_{m-1}(P_{\perp\mathbf{u}^{(k)}}(A - \gamma^{(k)}I)P_{\perp\mathbf{u}^{(k)}}, \mathbf{r}^{(k)})$ . The  $\mathcal{K}_m(A, \mathbf{u}^{(k)})$  can be used to compute an approximate eigenvalue for  $\gamma^{(k)}$ , while  $\mathcal{K}_{m-1}(P_{\perp\mathbf{u}^{(k)}}(A - \gamma^{(k)}I)P_{\perp\mathbf{u}^{(k)}}, \mathbf{r}^{(k)})$  can be used to compute an approximate solution  $\mathbf{t}_*^{(k)}$  of the linear equation (6) (initial guess is supposed to be  $\mathbf{0}$ ).

From this observation, we consider an approach to the correction vector: we generate the Krylov subspace  $\mathcal{K}_m(A, \mathbf{u}^{(k)})$ ;

- not only to compute an approximate eigenvalue for  $\gamma^{(k)}$  in (6) by using the Krylov subspace  $\mathcal{K}_m(A, \mathbf{u}^{(k)})$ ;
- but also to compute an approximate solution  $\mathbf{t}_*^{(k)}$  of (6) by using the Krylov subspace  $\mathcal{K}_{m-1}(P_{\perp\mathbf{u}^{(k)}}(A - \gamma^{(k)}I)P_{\perp\mathbf{u}^{(k)}}, \mathbf{r}^{(k)})$ .

In this way, we can use the two Krylov subspaces for the correction vector by generating only one Krylov subspace. Finally, an approximate solution of (6) is orthonormalized against the basis of  $\mathcal{Q}_k$ , and then the resulting vector is the next basis vector to expand  $\mathcal{Q}_k$ .

### 4 Numerical experiments

Computational environment is MATLAB (version 7.10.0.499 (R2010a) 64bit) run under Linux with Intel Core i7-3770S (3.1 GHz). In all experiments, an initial vector is  $\mathbf{u}^{(1)} = [1, \dots, 1]^T / \sqrt{n}$ , and iterations stop if  $\|\mathbf{r}^{(k)}\| \leq 10^{-10}$ .

We consider the eigenvalue problem of an  $n \times n$  real nonsymmetric matrix

$$A = \begin{bmatrix} a_1 & a_3 & & & 0 \\ a_2 & a_1 & a_3 & & \\ & \ddots & \ddots & \ddots & \\ & & & & a_3 \\ 0 & & & a_2 & a_1 \end{bmatrix},$$

of which the eigenvalues are

$$\lambda_j = a_1 + 2\sqrt{a_2 a_3} \cos \frac{j\pi}{n+1} \quad (j = 1, \dots, n).$$

The following methods are compared.

**JD:** The JD method using 10 steps of GMRES.

**JD $\star$ :** The new version of the JD method with  $m = 11$ .

Note that these methods require 10 matrix-vector multiplications to generate a basis vector per iteration. The problems are determined as follows.

- (a) The target is the largest eigenvalue  $\lambda_n$  for  $n = 100$ ,  $a_1 = -2.0$ ,  $a_2 = 1.0$ , and  $a_3 = 1.6$ .
- (b) The target is the eigenvalue closest to  $-2.1 + 0.1i$  for  $n = 100$ ,  $a_1 = -2.0$ ,  $a_2 = 1.0$ , and  $a_3 = 0.9$ , which is the interior eigenvalue  $\lambda_{52}$ .

We show the convergence history of the residual norm  $\|\mathbf{r}^{(k)}\|$  in Fig. 1. From Fig. 1, we observe that JD $\star$  converges slightly faster than JD in the both cases (a) and (b).

## 5 Concluding remarks

To generate a subspace, we have focused on approximate solving a linear equation which is known as a correction equation. The equation is determined by an approximation of a wanted eigenvalue, and a good approximation is appropriate to find the eigenvector which corresponds to the wanted eigenvalue in the subspace.

In this report, we have considered utilizing an invariance of Krylov subspaces to use one Krylov subspace for two aims. The first aim is to generate approximate eigenvalues that determine correction equations. The second aim is to solve the equations approximately. By the choice of a correction equation and its approximate solution, we have proposed a new version of the

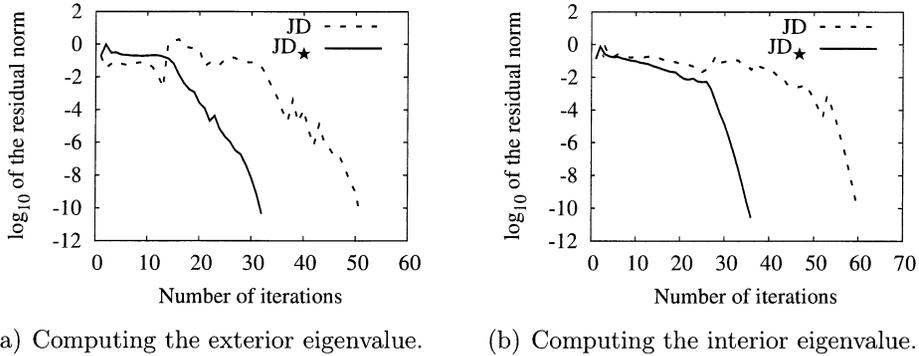


Figure 1: The convergence history of the residual norm.

Jacobi–Davidson method. In the new method, a better approximated eigenvalue can be put into the correction equation, while keeping the number of matrix-vector multiplications per iteration the same as the Jacobi–Davidson method. Numerical experiments show that the new method has attractive convergence behavior in comparison with the Jacobi–Davidson method. Therefore, we conclude that the new version of the Jacobi–Davidson method is promising for computing a few eigenpairs of a large sparse matrix.

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